Simulation Standard

Connecting TCAD To Tapeout

A Journal for Process and Device Engineers

Simulating Solar Cell Devices Using Silvaco TCAD Tools

1. Introduction

Silvaco TCAD offers complete and well integrated simulation software for all aspects of solar cell technology. TCAD modules required for Solar Cell simulation include: *S-Pisces, Blaze, Luminous, TFT, Device3D, Luminous3D and TFT3D* [1]. The *TCAD Driven CAD* approach provides the most accurate models to device engineers. Silvaco is the one-stop vendor for all companies interested in advanced Solar Cell technology simulation solutions.

2. TCAD Modules For Solar Cell Technology Simulation

Brief descriptions of the TCAD modules that can be used for solar cell technology simulation are listed below. For more details of these modules, please visit the Silvaco TCAD products website [2].

S-Pisces is an advanced 2D device simulator for silicon based technologies that incorporates both drift-diffusion and energy balance transport equations. Large selections of physical models are available for solar cell simulation which includes surface/bulk mobility, recombination, impact ionization and tunneling models.

Blaze simulates 2D solar cell devices fabricated using advanced materials. It includes a library of binary, ternary and quaternary semiconductors. *Blaze* has built-in models for simulating state-of-the-art multi-junction solar cell devices.

Device3D is a 3D device simulator for silicon and other material based technologies. The DC, AC and time domain characteristics of a wide variety of silicon, III-V, II-VI and IV-IV devices be analyzed.

Luminous and *Luminous3D* are advanced 2D and 3D simulator specially designed to model light absorption and photogeneration in non-planar Solar Cell devices. Exact solutions for general optical sources are obtained using



Figure 1. Spectral Response of a Solar Cell.

geometric ray tracing. This feature enables *Luminous* and *Luminous3D* to account for arbitrary topologies, internal and external reflections and refractions, polarization dependencies and dispersion. *Luminous* and *Luminous3D* also allows optical transfer matrix method analysis for coherence effects in layered devices. The beam propagation method may be used to simulate coherence effects and diffraction.

*TFT*land *TFT3D* are advanced 2D and 3D device technology simulators equipped with the physical models and specialized numerical techniques required to simulate

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Figure 2. Photogeneration Contours in Amorphous Silicon Solar Cell Device.

amorphous or polycrystalline devices including thin film transistors. *TFT* and *TFT3D* can be used with *Luminous* and *Luminous3D* to simulate thin film solar cells made from amorphous silicon. Spectral, DC and transient responses can be extracted.

3. Simulating of Solar Cell Characteristics

Here, we will discuss the various aspects of solar cell characteristics that can be simulated by Silvaco TCAD tools. Typical characteristics include collection efficiency, spectral response, open circuit voltage, VOC and short circuit current ISC. Figure 1 shows the simulated spectral response of a solar cell using the *Luminous* module. This figure is obtained by varying the incident wavelength of



Figure 3. Photogeneration Rate from Angled Light Beam.



Figure 4. Solar Cell with Texture Surface.

a light source to extract the solar cell's spectral response. From this figure, the green curve is the equivalent current from the light source; the red curve is the available photo current generated by the light within the solar cell device and the blue curve is the actual terminal current. Collection efficiency inlcuding the effects of reflection can be caluclated by the ratio of these quantities.

It is possible to study the details of photo generation of carriers in the solar cell device during light illumination. This is very useful for simulation of multi-junction devices. Figure 2 shows an elevated contour plot of photogeneration rate in a simple thin film amorphous silicon solar cell. Note that in this figure, the device has an opaque metal contact in the center of the structure. Once photogeneration rates are obtained, terminal currents can be evaluated to determine the quantum efficiency of the solar cell.

One useful feature of the *Luminous* module is ray tracing. This feature enables the analysis of more advanced solar cells designs. Besides studying the photogeneration rates due to a normal incident light beam, the photogeneration rates due to an angled light beam can also be studied. This is shown in Figure 3.

For large area solar cell devices, the surface of the cell will take the shape of inverted cone, pyramid, etc (depending on the type of optics). Figure 4 shows the photogeneration in a silicon solar cell when light impinges on the cell which has pyramids on the surface. From this figure, it can be seen that the light path inside the semiconductor is diverted from its original path due to the pyramid surface. This causes the contour of the photogeneration rates to be a saw-tooth shape as shown in the right hand side of Figure 4.



Figure 5. Current Voltage Characteristics of Amorphous Silicon Solar Cell Device.

Once the photogeneration rates are obtained by the *Luminous* module, *ATLAS* will then be able to simulate the terminal currents to obtain the IV characteristics. Figure 5 shows the IV characteristics of an amorphous silicon solar cell under AM0 illumination. In this figure, ISC is the short circuit current and VOC is the open circuit voltage. The ISC is extracted from the curve when the voltage is zero. On the other hand, the VOC can be extracted from the IV curve when the current is zero. Also, the maximum current, Im and maximum voltage, Vm, can be obtained from the maximum power rectangle as indicated in the figure.

By changing the illumination power of the light beam, we can obtain a series of IV characteristics as a function



Figure 6. Amorphous Silicon Solar Cell Simulation with Different Light Power.



Figure 7. Potential Distribution in a Solar Cell.

of the illumination power can be obtained. This is shown in Figure 6. From this figure, it can be seen that the short circuit current increase linearly with the increase of light power, where the open circuit voltage begins to saturate with the increase of light power.

Three-dimensional simulation of solar cells can be performed to investigate effects such as electrical losses in the cell structure due to variation in the front metal grid finger geometry. In such cases, it is necessary to use *ATLAS3D* together with the 3D modules for solar cell simulation. Figure 7 shows the 3D structure of a large area solar cell device. The potential distribution in the solar cell device after the light illumination is displayed in this figure.

4. Conclusion

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 Threedimensional domains. The simulated properties include IV characteristics, spectral response, quantum efficiency, photogeneration rates, potential distribution, etc. In addition, the software is also capable of simulating amorphous silicon solar cell devices and large area solar cells with texture surfaces. Silvaco is the one-stop vendor for all companies interested in advanced solar cell technology simulation solutions.

References

1. "ATLAS User's Manual", Silvaco, Santa Clara, California, USA.

2. Silvaco ATLAS website: http://www.silvaco.com/products/device_ simulation/atlas.html

TCAD TFT AMLCD Pixel Simulation

1. Introduction

The main drawbacks of circuit level simulation are the many assumptions made of the device model. For example the a-Si:H TFT model assumes that the channel is uniform and ignores interface trap effects. For more accurate circuit level simulation, a device numerical modeling approach is attractive and predictive. Silvaco's *ATLAS/MixedMode* module enables users to predict device performance and also the circuit level behavior of transient switching characteristics in AMLCD pixel simulation. Figure 1 shows conventional equivalent circuit diagram of the unit pixel.

2. Liquid Crystal Capacitance Model

In order to simulate transient behavior of the unit pixel in *MixedMode*, a time and voltage dependent liquid crystal capacitance model is to be used.

$$\varepsilon_{ps} = \varepsilon_{PL} + \delta \cdot \gamma \cdot \exp(D_{time}) \cdot \sqrt{\frac{V}{V_C} - 1}$$

The total amount of LC capacitance(C_{LC}) is calculated from above ε_{ns} and the geometry of the LC cell as follows:

$$C_{lc} = \frac{\varepsilon_0 \cdot \varepsilon_{ps} \cdot L \cdot W}{D}$$

here, L and W are total area of the LC cell which is connected to each TFT and D is the thickness of the LC cell(cell gap).

The parameters used in the simulation are listed in Table 1.

Liquid Crys	stal Parameters
L	=152um
W	=148um
D	=10.02um
δ	=51.0 mm²/s
γ	= 51.2 ms/mm ²
D_{time}	= 100ms
Vc	=1.887V
e _{PL}	=3.1

Table 1. LC parameters in *MixedMode* simulation.



Figure 1. This figure shows AMLCD unit pixel.

3. MixedMode Circuit Description

In order to simulate liquid crystal capacitance with *MixedMode*, a user-defined two terminal function with C-Interpreter is necessary.

Bxxx n+ n- infile="filename" function="function_name"

Bxxx is a user-defined name and infile="filename" is the source file which includes the function name.

An example C-Interpreter source file is listed below.

```
#include <math.h>
#include <math.h>
#include <stdio.h>
double my_lc_rc(double v, double temp,
    double ktq, double time, double *curr,
    double *didv, double *cap, double
    *charge)
{
    double eps,e0;
    double epl,clc;
    double theta,gamma;
    double Dtime;
    double L,W,D;
    L=152;
```

```
W=148;
Dtime=100e-3;
theta=51.0; /* sec */
```

```
gamma=51.2e-3; /* sec */
epl=3.1;
vc=1.887;
D=10.02;
e0 = 8.854e - 12;
if(v > vc)
     eps = epl + theta*gamma*exp(Dtime)*
sqrt(v/vc - 1.0);
else if( v <= vc)
     eps =epl;
clc= e0*eps*L*W*1e-6/D; /* F */
*curr=v/10e9;
*didv=1/10e9;
*cap=clc;
*charge=*cap*v;
printf("clc = e(F) n'', clc);
printf("charge = e n'', *charge);
return(0);
```

In the calculation above, a user-defined two terminal current is defined by the following formula:

```
I=F1(V,t) + F2(V,t)*dF/dV
```

}

The 1st term is the DC current and the 2nd term is the capacitive current.

MixedMode performs capacitance and total charge calculation based on the user-defined C-Interpreter function. A typical voltage driven response of unit pixel is shown Figure 2.



Figure 2. A typical TFT AMLCD unit pixel voltage driven response.

Before transient simulation in *MixedMode*, the DC characteristics of the a-Si:H TFT is simulated to reproduce the experimental transfer curve and output curve.

Interface traps are specified for the bulk and front and back channel using continuous DEFECT and INTDE-FECT statements. Interface fixed charge is also included.

In a TFT-LCD pixel simulation, the following a-Si:H TFT model and circuit behavior should be considered:

- 1. the charging state which is driven by the on-current of an a-Si:H TFT
- 2. the holding state which is affected by the off-current of an a-Si:H TFT
- 3. the voltage drop characteristics of an a-Si:H TFT and LC capacitance

The *MixedMode* circuit description input deck is listed below:

.begin

```
vcom 6 0 5
```

vg 1 0 0 pulse 0 20 0 1e-6 1e-6 40us
180us
vd 3 0 0 pulse 0 10 0 1e-6 1e-6 160us
320us
atft 2=source 1=gate 3=drain infile=a-SiTFT.str width=41

```
____
```

```
re 2 4 1.28k
```

co 4 5 317f

rlc 5 6 10g

cst 2 6 1.06p

#clc 4 0 125f

bLC 5 6 infile=lc_cap.lib function=my_lc_
rc

.numeric vchange=0.5 dtmin=1e-9 imaxtr=50
.options print
.load infile=tft_dc
.log outfile=tft

```
.tran 0.1us 320us
```

.end

In Figure 3, the AMLCD pixel dynamics are correctly reproduced, accordingly the source voltage shape shows pixel charging, holding, and voltage drop.

5. Conclusion

ATLAS/TFT/MixedMode is a useful tool for TFT AMLCD unit pixel simulation and predicts transient pixel characteristics with trap density of a-Si:H TFT and liquid crystal modeling through a user-defined two terminal device.

TCAD approach to pixel design and combined device level capacitance characteristics is necessary for both circuit and device performance.

References:

- "Dynamic Characterization of a-Si TFT-LCD pixels", Hitoshi Akoi,ULSI Research Laboratory, HP Labs, Hewlett-Packard Company, 3500 Deer Creek Rd., Palo Alto, CA 94304
- 2. "ATLAS User's Manual", Silvaco, Santa Clara, California, USA.



Figure 3. TFT AMLCD pixel voltage.

Material Modeling of Resistive Switching for Non-Volatile Memories Using ATLAS C-Interpreter/Giga

1. Introduction

Recently, a variety of materials having large non-volatile resistance change have been studied as potential candidates for next generation non-volatile memory devices. For example, chalcogenides for PCM (Phase-Change Memory) [1] and perovskite oxides or transition metal oxides for RRAM (Resistive Random Access Memory) [2] etc.

The basic operation of these devices is as follows: there are two states, RESET and SET. The RESET state is a high resistance state obtained by applying a sufficiently high electrical pulse to change crystal phase to amorphous phase for PCM, or to break the conduction path for RRAM. The SET state is a low resistance state obtained by applying a lower and longer pulse to change amorphous phase to crystal phase or to re-form conduction path.







Figure 2. Mobility change at initial, 50ns, 150ns and 200ns.

2. A Simple Material Model for Resistive Switching Operation

The detailed mechanisms of the resistive switching especially for RRAM materials are still under investigation, so developing better models which can account for experimental I-V curves of these devices are useful for comprehending the operation and optimizing both the operation and structure of the device.

For that purpose, the *C-Interpreter* is very helpful. It enables the user to create their own models in order to investigate material and device behavior.

For example, assuming that the phase change or conduction path destruction/re-formation is dependent on the material's temperature and its resistivity change can be expressed as a mobility change, a user-definable temperature dependent *C-Interpreter* mobility model can be used. The Giga module is used to account for selftreating effects.

Figure 1 is an example in which the mobility is described as a function of temperature, depending on the range and the direction of the temperature and mobility change.

3. Simulation Results

The device structure simulated is very simple as shown in Figure 2. A resistive switching material with the user defined mobility model is sandwiched between two electrodes. A bipolar triangular voltage sweep of 200ns shown is applied as shown at the top of Figure 3.



Figure 3. (Top) Triangular voltage sweep applied. (Middle) A temperature change at a point near the center of the device. (Bottom) Mobility change at that point.

Figure 2 shows the mobility change in an applied voltage cycle. The top left picture is the initial SET state of high mobility. The top right picture shows the mobility and temperature contours at 50ns, the mobility decrease depends on the temperature distribution, and corresponds to a phase change from crystal to amorphous or to the breaking of conduction path. The bottom left picture at 150ns shows that the mobility increases again; the increase corresponds to re-crystallization or re-formation of the conduction path. The bottom-right is the state at 200ns in which mobility is kept at the SET state once reached at 150ns.

The mobility and temperature near the device center at X=0.6um Y=0.5um traced for one cycle are shown in Figure 3. The I-V hysteresis curve of the device is shown in Figure 4. A typical hysteresis curve can be obtained by the simple temperature dependent mobility functions defined in Figure 1.

4. Conclusion

When conventional models are not applicable for new material devices, it is useful to develop a user defined model using the *C-Interpreter*. It provides users with a flexible method to comprehend the device behavior and to optimize its operation and structure.



Figure 4. Simulated I-V hysteresis loop for one cycle.

References

- S.Lai, T. Lowrey, "OUM-A 180nm nonvolatile memory cell element technology for standalone and embedded applications", IEDM Tech., Dig., 2001, pp. 36.5.1 - 36.5.4
- Y.Hosoi, et al., "High Speed Unipolar Switching Resistance RAM(RRAM) Technology", IEDM Tech., Dig., 2006, pp.30.7.1 -30.7.4.

Hints, Tips and Solutions

Stephen Wilson, Applications and Support Engineer

Q. How do I create Circular and Cylindrical meshes in ATLAS ?

A. It has been possible for some time to create meshes with circular and cylindrical symmetry using the *DevEdit* device building tool. This capability has been extended recently to the *ATLAS* command language, thus providing the *ATLAS* user with an alternative and more convenient way to construct devices with circular symmetry. Possible applications are nanowires and mesa-type structures. For nanowires, quantum transport models are available.

To specify a circular mesh with *ATLAS2D*, the user includes the parameter CIRCULAR on the MESH statement. The properties of the MESH must then be given by using a number of R.MESH and A.MESH statement. The radial mesh spacing is controlled by the R.MESH statements, and the angular mesh given by the A.MESH statements.

To conform to the new MESH shape , the parameters R.MIN, R.MAX, A.MIN, and A.MAX have been added to the REGION, ELECTRODE and DOPING statements.

 Deckbuild V3.36.0.R – ect1.in, dir; 	100
$\fbox{Fils } \tau) \underbrace{ \texttt{View } \tau } \underbrace{ \texttt{Edit } \tau } \underbrace{ \texttt{Finc } \tau } \underbrace{ \texttt{Main Cortrol } \tau } \underbrace{ \texttt{Corr mands } \tau } \underbrace{ \texttt{Tools } \tau }$	(T)
_mesh_circ_lar *.r=1=0.0 spac=0.05 r.r=1=0.8 spac=0.1 r.r=1=1.2 spac=0.1	14
ε.π 1=0 spε<=22.5 ε.π 1=3€0 spε<=22.5	
region rum=1 məterr∋l≕vacuum almin=0 almax=360.0 r.max=0.8 region rum=2 məterrəl≕cxidə r.min=0.3 r.məx=0.8 region rum=3 məterrəl=arr r.min=0.5 r.max=1.1	
ejectroce name=gate a.min=20. p.mex=22.5 r.min=0.5 r.mex=1.0 ejectroce name=gate1 a.min=45 p.mex=67.5 r.min=0.5 r.mex=1.0 ejectroce name=gate2 a.min=30 p.mex=157.5 r.min=0.5 r.mex=1.0 ejectroce name=gate3 a.min=180 p.mex=157.5 r.min=0.5 r.mex=1.0 ejectroce name=gate4 a.min=180 p.mex=247.5 r.min=0.5 r.mex=1.0 ejectroce name=gate3 a.min=225 p.mex=247.5 r.min=0.5 r.mex=1.0 ejectroce name=gate7 a.min=215 p.mex=247.5 r.min=0.5 r.mex=1.0 ejectroce name=gate7 n.min=315 p.mex=347.5 r.min=0.5 r.mex=1.0	
method carrier=0	
save outf=ect1.str	
solve in t	
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(rext) line cont qu t Line:	1
(paste) (init) (pause) (clear) restart (kil) Stop:	Non

Figure 1. Example ATLAS commands for the electrical capacitance tomography cell.

These permit the use of polar coordinates in delineating the edges of REGIONS and ELECTRODES. The minimum radius is specified by R.MIN and the maximum by R.MAX, both in units of microns. A.MIN and A.MAX specify the minimum and maximum angular ranges respectively, in units of degrees between 0 and 360.

To give a first example, for illustrative purposes only, the set of *ATLAS* commands shown in Figure 1 results in the structure as shown in Figure 2. For best results the radial limits of the REGIONS and ELECTRODES align with R.MESH locations, and the angular limits align with the major spokes as defined by the A.MESH spacing.

In some cases it may be possible to study a reduced angular range, rather than a full circle. For this reason the MAXANGLE parameter has been introduced onto the MESH statement to allow the user to specify a wedge shaped device structure. MAXANGLE should not be greater than 180 degrees. The algorithm used by MESH CIRCULAR creates a constrained Delaunay mesh. If the radial mesh spacing decreases with increasing radial position, obtuse elements can sometimes be created. The number of obtuse elements can typically be reduced by the use of the MINOBTUSE parameter, also on the MESH statement.



Figure 2. Circular device structure for Electrical capacitance tomography cell.



Figure 3. Example ATLAS commands for a semi-circular structure.







Figure 5. Doping density in semi-circular structure showing p-n junctions.

The R.MIN, R.MAX, A.MIN and A.MAX parameters have also been implemented for the DOPING statement. They apply to the analytic doping profiles, UNIFORM, GAUSSIAN and ERFC. For GAUSSIAN and ERFC doping profiles the principal direction is the radial direction and the lateral direction is the tangential direction. Figure 3 shows the use of these parameters.

This gives a semi-circular structure as shown in Figures 4 and 5. The doping density along with junction positions are also shown.

Of arguably more use is the ability to create cylindrical structures in *ATLAS3D*.

This is effected by using the CYLINDRICAL parameter on the MESH statement in ATLAS3D. A distinction must be made between the structures produced by ATLAS2D and ATLAS3D when using the CYLINDRI-CAL parameter. In ATLAS2D, the Device is a body of revolution around the x=0 axis, and consequently has no angular dependence. In *ATLAS3D*, using the CYLINDRICAL parameter allows a device with full radial, angular and axial variations to be modelled. To achieve this both the REGION and ELECTRODE statements accept the R.MIN, R.MAX, A.MIN and A.MAX parameters as well as the Z.MIN and Z.MAX parameters. The DOPING statement also accepts these parameters for analytical doping profiles. The principal direction of the doping is in the z-direction, with the parameters CHAR, PEAK, DOSE, START and JUNC-TION applying to the z-direction. The lateral fall-off in the radial and angular directions can be controlled

File Edit Apps Options Buffers Tools
Com Deci See Met of app Park Loss See Holes Hill Pr Nos Vider
nesh three d cylindrical max.angle=90 0 minobtuse
r.m 1=0.0 spac=0 5 r.m 1=0.5 spac=0 25 r.m 1=0.6' s spac=0.035 r.m 1=1.65 spac=0.035 r.m 1=1.65 spac=0.25 r.m 1=2.25 spac=0.25 r.m 1=2.3 spac=0.05
a.m 1=0.0 spac=36 0 a.m 1=360.0 spac=36.0
$ \begin{array}{llllllllllllllllllllllllllllllllllll$
region number=1 r max=2.3 material=si ⁺ icon region number=2 r min=0.615 r.max=0.65 z.max=1.7 material=oxide region number=3 r min=0.05 r.max=0 65 z.min= ⁺ .7 z.max=5.3 material=oxide region number=4 r min=1.65 r.max=2 3 z.min=0.2 z.max=9.1 material=oxide region number=6 r min=1.65 r.max=2 3 z.min=0 z.max=9.1 material=oxide region number=6 r min=2.25 r.max=2 3 z.min=5 3 z.max=9.1 material=oxide
electrode name=gate r.max=0.615 z.max=1.7 electrode name=gate1 r.max=0.5 z min=1.7 z max=5.3 electrode name=gate3 r.min=2.25 r max=2.3 z max=5.3 electrode name=source r.min=0.65 r max=1.65 z.max=0.5 electrode name=drain z.min=9.1 z.max=9.5

Figure 6. Example ATLAS commands for the cylindrical wedge structure.



Figure 7. Example cylindrical structure.

by the LAT.CHAR or RATIO.LAT parameters. An example of a quite complicated 3d cylindrical geometry produced by the commands shown in Figure 6, is shown in Figure 7.

The MAXANGLE parameter has been set to 90 degrees, but the major angular spacing is 36 degrees. *ATLAS* requires that the actual MAXANGLE used correspond to a whole number of major angular mesh spacings. Thus the mesh spacing has been automatically corrected by *ATLAS* to 108 degrees. This can be seen in a cutplane of the structure.

Tip : Because the mesh is independent of position along the z-axis, the radial and angular boundaries of all the RE-GION's and ELECTRODE's are included in the R.MESH and A.MESH statements, irrespective of the z-location of the REGION. It is always recommended to have mesh points exactly co-incident with region boundaries.



Figure 8. Cutplane of Cylindrical structure, showing details of mesh.

Call for Questions

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