Among the many design criteria for solar cells, the design of the top metal contact impacts the cell efficiency. The areal density of the top contact modifies the magnitude of the cell output power significantly.

Solar cells suffer from optical losses. These limit the total number of photogenerated carriers. Add to that, carriers suffer from electronic (recombination) losses. Using numerical simulations these losses can be quantified and minimized.

Photogenerated carriers experience bulk resistivities as well as surface sheet resistivity before collection at the top contacts. The contact design aims to maximise carrier collection against internal resistance and metal shadowing. For complex metal designs there are no simple analytical solutions for the optimum contact areal density. In this article, 3D TCAD software is used to maximise the cell output power as a function of contact areal density.

**Solar Cell Losses**

The design of the top contact aims to reduce the fractional power loss [1] which is defined as:

\[ f_{\text{loss}} = \frac{\rho_s}{J_{mp}} \cdot \frac{V_{mp}}{P_{max}} \]

where \( \rho_s \) is the sheet resistivity, \( J_{mp} \) is the maximum power current density and \( V_{mp} \) is the maximum power voltage.

High contact areal density reduces the impact of the surface sheet resistance but increases the shadowing. On the other hand a low contact density will reduce the shadowing effect boosting the generation power but increases the losses due to the sheet resistance.

TCAD numerical modelling of the various metal coverage ratios helps to locate the optimum contact design density.

**Simulation Setup**

A simple silicon solar cell with top p-type contacts (cathode) and an n type bulk with back substrate contact is used. A cell of 4 mm² and 100 micron thick was created using Victory Process (Cell Mode) employing a mask set for the implants and metallization layer. A simple basic process flow involving two implants and anneal steps as well as the Aluminium metallization for the top contacts was used.

The process simulation contain less than 20 steps. Following the `init` statement, `line` statements were used to control the volume data resolution. For this study, the x and y lines, which defined the surface plane, had uniform spacing, while z was set with small spacing near the top and bottom surfaces and larger spacing in the middle. The idea is to capture the doping profile near the surface. In total 201 x 201 x 39 lines were generated. This generates a structure in excess of 1.575 million points. Nevertheless, the simulations ran in less than 4 hours and 15 minutes on a single CPU. The main overhead was due to the diffusion steps.

At the end of the process simulation, the `export` statement was used to generate a structure suitable for the device simulations. Users have a number of options here. In this study conformal and Delaunay mesh export were investigated.

Since this is a large solar cell structure of 4 mm² or 4 million \( \mu \text{m}^2 \), careful device meshing of the final structure suitable for the Victory Device simulation was needed. The conformal meshing algorithm generated more than 1.2 million nodes and 70 million tetrahedral, while the Delaunay mesh algorithm produced 65k nodes and less than 300k tetrahedral. For the Delaunay mesh adaptive refinement based on the distance to the p-n junction was used. This leads to a significant speed up of the device calculations.

This adaptive refined meshing algorithm ensures an optimal density to speed up the device carrier generation and recombination and transport calculations. A typical Delaunay based Victory Device calculations took 20 minutes using 3 CPUs on a 4 CPU machine. This represents a speed up of x100 compared to the calculation involving the equivalent conformal structures with no adaptive refinement on the same machine and resources. Although there was a difference of 15% between the Isc from the conformal and Delaunay mesh structures, the maximum obtained power was within 2%.

![Figure 1. Showing the adaptive meshing used for the 4mm² solar cell.](image)
On the other hand, higher Delaunay mesh densities did not significantly impact the output data and produced short circuit currents $I_{sc}$ that were within 0.4% of the original values. This confirms that the Delaunay meshing density used did not significantly impact the precision of the final result.

For the Aluminium top contact, a regular hexagonal grid mask was used. This shape which is characterized by six equal sides and internal angles of 120°, provides uniform top surface coverage and a simple method to characterise the exposed silicon to metal area ratio as described below. No suggestion is made here that hexagon grid contacts are the optimum design for such cells. In fact many more complex designs have been referenced in the last few years in the open literature [2].

Once the mask set is created, this is invoked in the process simulator Victory Process on the `init` statement. To generate a valid simulation matrix all parameters were kept constant apart from the size (and hence areal density) of the hexagons covering the top surface. This can be achieved easily using MaskViews.

It is a trivial step to expand or shrink the size of the hexagons to facilitate this study using MaskViews software. Load the mask set (.lay format in this case) into MaskViews, then use options => rescale layout then save.

This will change the area and density of the hexagon metal. However, associated with this action, the width of the Aluminium hexagon sides will also be modified. Since the aim here is to investigate the effect of the polygon areas on the cell efficiency, the metal finger widths need to be kept constant. To achieve this, the parameter “deltacd” was used on the `mask` statement in Victory Process. This critical dimension delta parameter offsets mask polygon edges by the defined number in microns. This made fixing the metal finger width a relatively trivial task.

An alternative approach useful for regular geometrical shape contacts such as used has been added in Version V 7.1.11 onwards. The new feature implemented on the `specifymaskpoly` statement allows users to convert circular shapes to regular polygons using “npoints” and “radius” to define the number of regular sides and the radius length.

The device calculations were performed using the Victory Device paralyzed linear iterative solver PAM. Raytracing was used to propagate the light into the solar cell. This robust algorithm is valid since no complex coherence effects were anticipated in the structure used in here. To expedite the calculations, the incoming beam was limited to a monochromatic beam with a wavelength of 0.6 μm. A full solar spectrum could be used which might produce more representative results. Nevertheless, the methodological approach remains the same.

Apart from setting the bulk carrier lifetime, surface recombination rate for both holes and electrons was set for the top surface using the interface statement.
Data Analysis

In order to compare the various cells used, the following coverage ratio was defined:

\[ R = \frac{A_{si}}{A_{al}} \]

Where is the area of the exposed silicon within a hexagon calculated as

\[ A_{si} = \frac{3\sqrt{3}}{2} a^2 \]

Here is the length of the side which is also the radius of the circumcircle that envelops the hexagon. On the other hand for the Aluminium,

\[ A_{al} = 6ab + c \]

Where \( A_{al} \) represents half the aluminium metal area surrounding the regular hexagons. Here \( b \) is half width of the metal fingers and \( c \) is an additional correction triangular areas at the six apex angles.

The ratio \( R \) values investigated in this study ranged from 40.3 to 4.3. This corresponded to the regular hexagon circumcircle radius of 935 \( \mu \)m to 104 \( \mu \)m.

Although other data is available that confirm the trend shown in here, the three structures used in this article can be characterized in the following table:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Small (high density hexagons)</th>
<th>Medium</th>
<th>Large (low density hexagons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Circumcircle diameter or hexagon side (micron)</td>
<td>104</td>
<td>450</td>
<td>935</td>
</tr>
<tr>
<td>Coverage ratio R</td>
<td>4.3</td>
<td>9.5</td>
<td>40.26</td>
</tr>
<tr>
<td>Plot color</td>
<td>Red</td>
<td>Green</td>
<td>Blue</td>
</tr>
<tr>
<td>Short Circuit current Isc (A)</td>
<td>0.014</td>
<td>0.016</td>
<td>0.017</td>
</tr>
<tr>
<td>Fill Factor</td>
<td>0.715</td>
<td>0.708</td>
<td>0.613</td>
</tr>
<tr>
<td>Maximum output power (mW)</td>
<td>6.6</td>
<td>7.4</td>
<td>6.8</td>
</tr>
</tbody>
</table>

In Figure 6 the light IV characteristics show a variation in the short circuit current \( (I_{sc}) \) but similar open circuit voltage \( (V_{oc}) \) of 0.65 volt was obtained as expected.

These cells produced similar open circuit voltage \( V_{oc} \) of about 0.65 V. Although the largest hexagon solar cell produces 6% more short circuit current \( I_{sc} \) the associated benefit is counteracted by 16% lower fill factor \( FF \) of 0.61 compared to a \( FF \) of 0.71 for the other two cells.

Since the solar cell efficiency is defined as

\[ \eta = \frac{I_{sc}V_{oc}FF}{P_{in}} \]

Figure 5. showing the largest and smallest hexagon grid top contact for the 1mm2 Silicon solar cell investigated in this study.

Figure 6. showing the solar cell IV with the red trace for the smallest hexagons (circumcircle radius or side length \( a \) of 104\( \mu \)m), green (\( a=225\mu \)m) and blue for the largest hexagon (\( a=945\mu \)m).
Figure 7. showing the PV sweep of the three solar cells. As before red (a=104μm), green (a=225μm) and blue (a=945μm).

It is clear that both factors carry the same influence on the overall conversion efficiency of the cell. This also explains how the maximum output power of the cells was greatest for the middle density cell with the coverage ratio of 9.5 as shown in Figure 7.

The green trace above shows an increase in the maximum cell power of 8% with respect to the blue trace and 11% with respect to the red trace.

Figure 8 is a plot of the cell output power as a function of the coverage ratio for the selected material and process flow used in this study. A clear maximum power peak is obtained for the silicon coverage ratio of 9.5.

Conclusion

In conclusion, numerical simulations allow solar cell designers to discover the optimum metallization aerial density for complex designs. 3D process and device TCAD simulations have been used to achieve this. Adaptively refined Delaunay meshing produced significant speed up with the device simulations.

This type of study can be easily driven via the Virtual wafer fab (VWF) design of experiment (DOE) matrix calculations. Finally, the new feature of the specifymaskpoly statement will allow users to automate the optimization of the top contact areal density. The size and in turn the aerial density of regular polygons can be defined in the deck for each iteration “on the fly”.

This opens up the possibility of using the powerful Silvaco automation tools to locate optimal designs.

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References


Figure 8. Showing the relationship between the maximum output power and the metal coverage ration R.