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Simulation of 3D Anisotropic Crystal Etching with VICTORY Process

1. Introduction

Anisotropic crystal etching is the common technique used in Micro Electromechanical systems (MEMS) manufacturing. It uses the property of some single crystal materials, like silicon, of having different etching rates in different crystal directions when the material is etched in special chemicals, such as potassium hydroxide (KOH). Predicting the resulting shape of the structure under such conditions requires full three-dimensional simulation of the evolution of the etched surface.

Silvaco's 3D process simulator VICTORY Process is perfectly suitable for such task. The numerical engine of VICTORY Process is able to accurately model physical etching with complicated distributions of etch rates over the surface even for initial structures with complex three-dimensional topographies.

2. Defining the Anisotropic Etch Rates

In order to model anisotropic crystal etching you have to specify

- a reference etch rate (in VICTORY Process this applies to the {100} crystal plane) and
- relative rates for the principal crystal axes.

Etching rates for intermediate directions are obtained by interpolation. VICTORY Process uses a linear interpolation as proposed in [1], which maintains C^0 continuity across the crystal planes. Note, that there is no need to demand higher order continuity, as it would prevent formation of sharp edges as observed in experiments [2].

When simulating anisotropic crystal etching, VICTORY Process takes into account the silicon crystal's symmetry. Therefore, it is enough to interpolate the etch rates not for the whole sphere (over all possible etching directions) but for its segment $0 \leq \theta \leq \pi/2$, $0 \leq \phi \leq \pi/4$ where θ and ϕ are elevation and azimuth in polar coordinates. This segment is divided into 'spherical triangles'. The number of spherical triangles which are used by the interpolation routine, depends on the number of the principal axis for which relative etching rates are provided in the input deck. Within each of those spherical triangles linear interpolation is used. See [1] for more details.

At the moment VICTORY Process allows user to specify relative etch rates either along

- 3 - ({100}, {110}, {111}) or
- 4 - ({100}, {110}, {111}, {311})

principal axis.

Within the input deck, you can provide those relative etch rates by means of the ETCHDEPOPROPERTIES statement. For example,

```
ETCHDEPOPROPERTIES name="KOH_3" \
   material="silicon" rate=0.797 \
     r100=1.0 r110=1.855 r111=0.0073 \
   material="resist" rate=0.00
```

defines etching properties for anisotropic crystal etching of silicon. The name 'KOH_3' is assigned to these properties so that they can be used (referred to) later on in the deck for performing the actual etching simulation. Those etching properties contain:

- the anisotropic etch rates for crystalline silicon
  - o with a reference etch rate in {100} direction of 0.797 *μm/min*

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- o with different rates in <u>two</u> other directions set as *Rate*{110} = 1.855**Rate*{100} and *Rate*{111} = 0.0073 * *Rate*{100}

- and the isotropic etch rate for resist of 0.00 $\mu m/min$

The statement:

```
ETCHDEPOPROPERTIES name="KOH_4" \
   material="silicon" rate=0.797 \
    r100=1.0 r110=1.855 r111=0.0073 r311=1.801 \
   material="resist" rate=0.00
```

defines etching properties which contain

- the anisotropic etch rates for crystalline silicon
  - o with a reference etch rate in {100} direction of 0.797 $\mu m/min$
  - o with different rates in <u>three</u> other directions set as *Rate*{110} = 1.855*Rate*{100} and *Rate*{111} = 0.0073 * *Rate*{100} and additionally for the plane {311} set as *Rate*{311} = 1.801*Rate*{100}
- and the isotropic etch rate for resist of 0.00 $\mu m/min$

The input deck name 'KOH_4' is assigned to those etching properties so they can be referred to later on in the input deck. Note that you can specify multiple etching properties within a single input deck. They may be valid for different processing conditions, like different temperatures.

The etching rates in the above examples are taken from [3] and correspond to the etching rates for silicon in a 30% solution of KOH at 70°C (note, that in the paper the reference direction is {110}).

It should also be noted here, that whenever you perform an anisotropic crystal etching, obviously, the wafer orientation and the wafer rotation, which you can set by means of the INIT statement by the parameters

- ORIENTATION
- ROT.SUB

are taken into account during etching.

3. Performing the Anisotropic Crystal Etching

Once you have defined the etching properties by means of the ETCHDEPOPROPERTIES statement, you can perform the actual anisotropic crystal etching step by calling the ETCH input deck statement as shown in Section 4. Within the ETCH input deck statement,

- You refer to previously defined etching properties by means of the parameter ETCHDEPOPROPERTIES
- Next you must select a model for etching simulation. The model which is suitable for anisotropic crystal etching is the "anisotropic" model
- You must also specify the etching time (in minutes by default in version 3.5.0.R) within the ETCH statement
- In order to optimize the numerical accuracy, we also recommend to set the SOLVER parameter, which selects the numerical scheme for moving the interfaces, to LAX_FRIEDRICH since this solver is more suitable for the etch rate profiles of anisotropic crystal etching than the default solver used in version 3.5.0.R of VICTORY Process
- Additionally you should also limit the size of the time steps by setting the parameter MAXCFL to 0.5 in order to minimize the numerical error of the solver which moves the interfaces

4. Examples

In all examples shown in this section we have used the etching properties as defined in section 2.

4.1 Specifying Etch Rates for 3 or 4 Principal Axis

The first example illustrates the effect of specifying the rate in the {311} direction in addition to the main {100}, {110} and {111} rates. We start from the structure shown on Figure 1 and etch it for 0.5 min using both etching properties "KOH_3" and "KOH_4" as defined in section 2.

The structures shown on Figures 2a) and 2b) are obtained by applying the commands

```
ETCH etchdepoproperty=KOH_3  \
     model="anisotropic" time=0.5 \
     maxcfl=0.5 solver=LAX_FRIEDRICH
```

and

```
ETCH etchdepoproperty=KOH_4 \
     model="anisotropic" time=0.5 \
     maxcfl=0.5 solver=LAX_FRIEDRICH
```

to the structure shown on Figure 1. You can see, that setting rates in 4 directions adds another facet to the etched surface, which is particularly visible on the hemisphere.

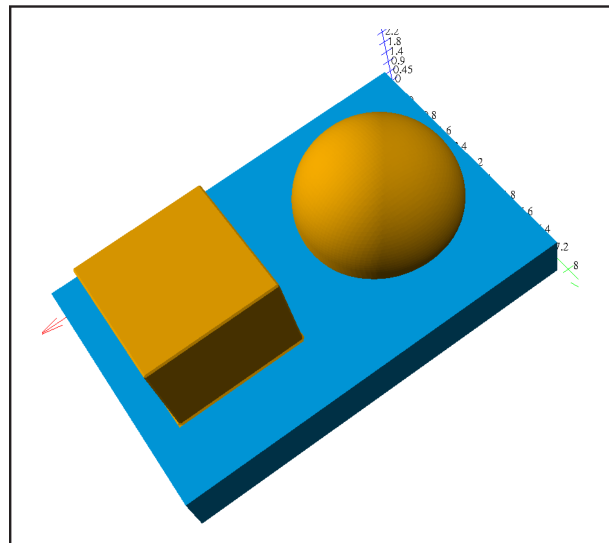
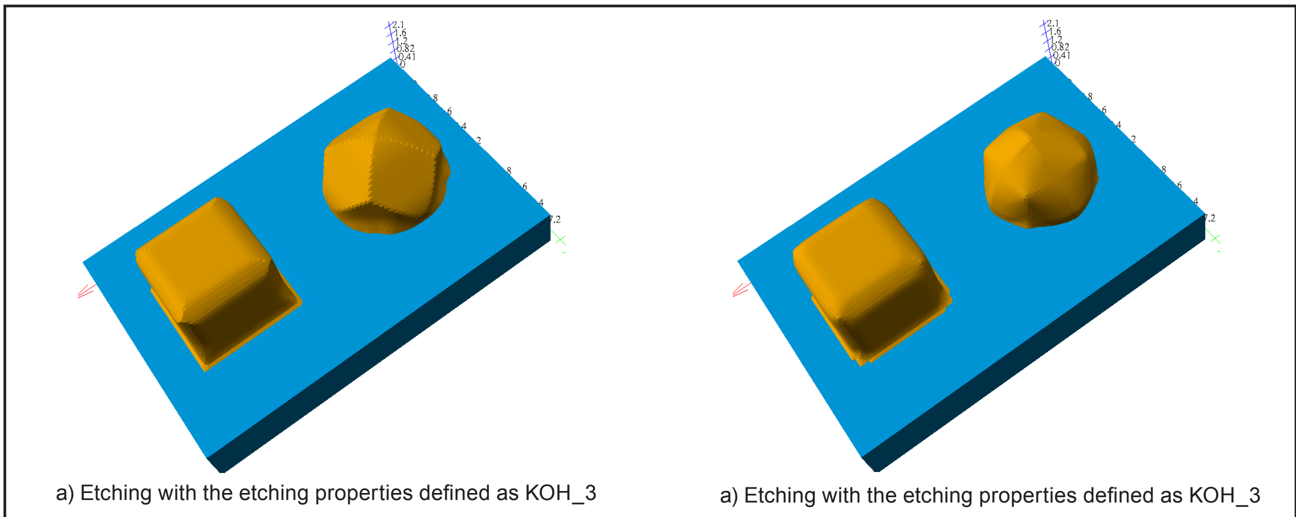


Figure 1. Initial structure.


a) Etching with the etching properties defined as KOH_3

a) Etching with the etching properties defined as KOH_3

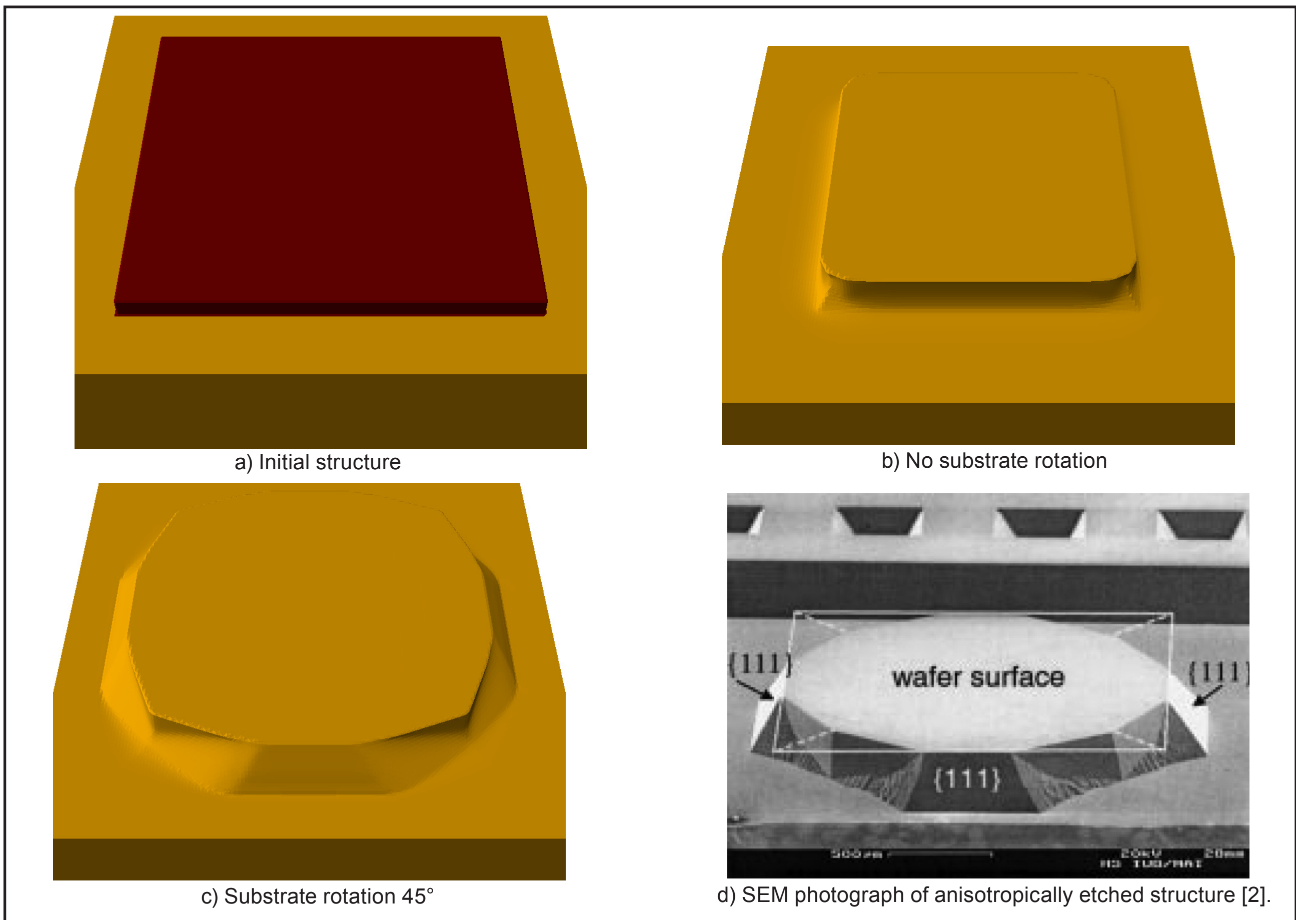
Figure 2. The difference between setting rates in 3 and 4 directions.

In the example shown in Figure 2 the default wafer orientation of version 3.5.0.R of VICTORY Process was applied. This means that:

- a {100} wafer (z-axis is {100} crystal direction) is used
- the wafer rotation is 0 degree (x-axis is {100} crystal direction).

4.2 The Effect of Wafer Rotation

The next example illustrates the effect of wafer rotation, which you can set in the INIT statement. Figure 3a) shows the initial structure. A silicon substrate with the square-shaped mask on the top is used for demonstration purposes. We have conducted two simulations with crystal anisotropic etching, whereby the same ETCH statement was applied.



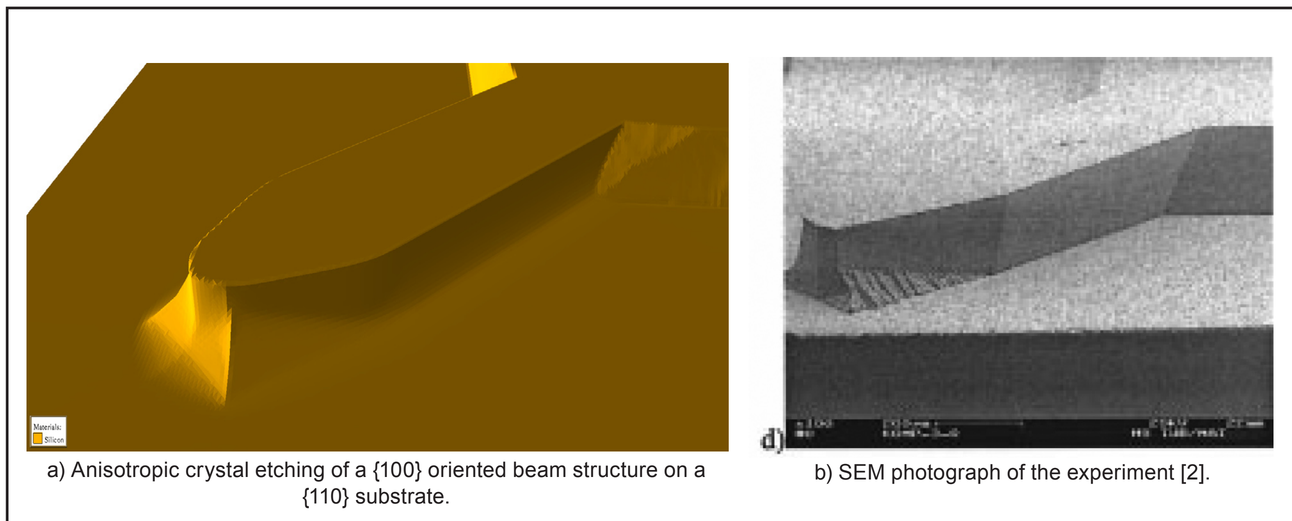
a) Initial structure

b) No substrate rotation

c) Substrate rotation 45°

d) SEM photograph of anisotropically etched structure [2].

Figure 3.Influence of the initial substrate rotation on anisotropic crystal etch and comparison with experimental results.



a) Anisotropic crystal etching of a {100} oriented beam structure on a {110} substrate.

b) SEM photograph of the experiment [2].

Figure 4. Comparison of simulation with experimental results.

```
ETCH etchdepoproperty=KOH_4 \
     model="anisotropic" time=2 \
     maxcfl=0.5 solver=LAX_FRIEDRICH
```

However, in first case the initial substrate was not rotated. Therefore, the mask's sides were aligned with the crystal direction {100}, while for second simulation the initial structure was generated with the parameter ROT.SUB set to 45° in the INIT statement. Although this does not change the visible shape of the initial structure it affects the position of the mask relative to the crystal's axis (as the crystal was rotated relative to domain's coordinate). That is why in the second case, the mask's edges were aligned with the {110} crystal direction.

As you can see in Figure 3, the rotation of the substrate had a dramatic effect on the resulting shape. Note, that substrate orientation and rotation can be set only at the beginning of the deck in the INIT statement and cannot be changed during the process simulation. In order to provide also a experimental verification, we have taken Figure 3d), from [2], where the SEM photograph of the structure as analyzed in this section, after anisotropic crystal etching is shown. The SEM image corresponds very well to the structure obtained by simulation (Figure 3c).

4.3 Etching of a Beam Structure

The last example in this article shows another comparison of simulation with experimental results for a frequently used benchmark. Anisotropic crystal etching is used to create a {100} oriented beam structure on {110} substrate.

Figure 4 shows very good agreement between simulated and experimentally obtained shapes.

5. Conclusions

VICTORY Process can accurately simulate the anisotropic crystal etching of silicon by setting the relative etch rates for different crystal directions. The results of simulation closely match experimental data.

Since anisotropic etching is a highly non-linear process, simulating it requires careful adjustment of the time step. We recommend to set the ETCH statement parameters MAXCFL to 0.5 or less and to use the LAX_FRIEDRICH solver for the etching process.

References

[1] Hubbard, *T.J, MEMS design: the geometry of silicon micromachining*, PhD thesis, California Institute of Technology, 1994.

[2] Schröeder, H. Obermeier, E., Horn, A., Wachutka, G.K.M. *Convex Corner Undercutting of {100} Silicon in Anisotropic KOH Etching: the New Strp-Flow Modl of 3-D Structuring and First Simulation Results.* J. of Microelectromechanical Systems, Vol. 10(1), 2001, pp. 88-97.

[3] Sato, K., Shikida, M., Matsushima, Y., Yamashiro, T., Asaumi, K., Iriye, Y., Yamamoto M., *Characterization of orientation-dependent etching properties of single-crystal silicon: effects of KOH concentration.* Sensors and Actuators A 64, 1998, pp. 87-93.

Extracting Concentrations from Arbitrary Shaped Well Regions

Introduction

It is often the case when simulating charged coupled devices (CCDs) or image sensors, that a designer wishes to know how many electrons or holes are contained within an arbitrary shaped n or p-well region for a given bias point or after exposure to light for a certain time and intensity.

The arbitrary shaped well will be defined by a metallurgic junction following all the process steps, usually simulated with the process simulator, ATHENA.

This article is for designers who feel that making the usual presumption that the well is rectangular in shape, will result in too great an error in the answer. If the well approximates to a rectangular shape, the usual area "Probe" statement will suffice. However, if the well has a very arbitrary shape, in order to obtain accurate numbers, we have to perform a numerical integration over the whole well shape. This numerical integration can be calculated using a series of extract statements inside a "LOOP" statement in the "Deckbuild" run time environment.

Example Structure

A simple example will be used to demonstrate the numerical integration technique. An N+ well region was created by implanting arsenic with a dose of 3e15/cm3 (70keV) and boron with a dose of 5e13/cm3 (15keV) into a mask with a 1um opening. The boron implant was required to define the metallurgic junction and give us another species to extract during the numerical integration.

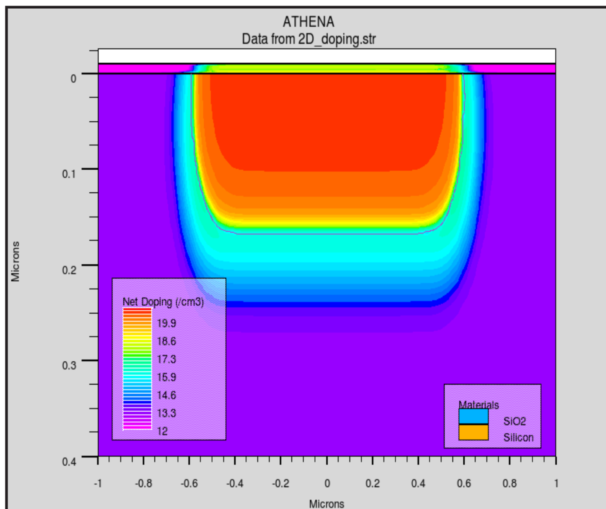


Figure 1. The N+ Well used to demonstrate the numerical integration technique.

The implants were then co-diffused for 20 minutes at 950 Centigrade to create a more arbitrary shape. The simple N+ well structure is shown in Figure 1.

Since we know how much arsenic and boron was implanted to create the well region, we should be able to predict the answer we get for the total number of arsenic and boron atoms in the well from the numerical integration technique to a reasonable level of accuracy. Any impurity can be extracted in the same way, such as electron an hole concentrations for example.

For a device of 1um width (1um in the "Z" direction), the total number of calculated arsenic atoms should be slightly less than:

The implanted dose (atoms/cm2) x surface area (cm2).

Since the mask opening and device width are both 1um, the simulated area is 1e-4 x 1e-4 = 1e-8cm^2 (1um = 1e-4cm). So the total number of arsenic atoms should be slightly less than

3e15/cm^2 x 1e-8cm^2 = 3e7 arsenic atoms.

Similarly, the total number of boron atoms should be slightly less than

5e13/cm^2 x 1e-8cm^2 = 500,000 boron atoms.

The reason we are expecting slightly less atoms than we implanted is because some of the implanted atoms will have diffused outside the boundary defined by the metallurgic junction (since the dopant boundary is not atomically abrupt). Since boron diffuses faster than arsenic, we would also expect a higher percentage of boron atoms to lie outside the junction.

Methodology

The method of numerical integration using the extract statements will slice the structure into horizontal bars, and integrate the species of interest between the first occurrence of the metallurgic junction in each slice and the second occurrence of the metallurgic junction in that same slice. The algorithm will then sum up the total number of the extracted species in all of the slices until it no longer finds any metallurgic junctions in a slice.

This basic method of integrating the number of a species in several slices bounded by metallurgic junctions can be modified for most shapes, even if this particular algorithm is not suitable for your particular shape.

Numerical integration in this case is simply the calculation of the area under the curve of the graph of concentration versus distance between the bounding metallurgic junctions for each slice. The complete integration is then the sum of the concentrations for all the slices.

Worked Example

The full extraction routine for the particular structure illustrated in figure 1 above is given below this paragraph. The purpose of each line will then be described. The user can then modify the various variables and details of the routine to suit their particular structure and species they wish to extract. In this example, two species are integrated within the well region, namely the total number of boron atoms and the total number of arsenic atoms, since these quantities are known.

Here is the complete extraction routine for both species:-

```
##### Numerical Integration Extraction Routine #####

set width=1
set depth=0.2
set steps=40
set increment=$depth/$steps
set yval=$increment/2.0
set totalarsenic=0.0
set totalboron=0.0

LOOP steps=$steps

extract name="j1" xj material="Silicon"
  mat.occno=1 y.val=$yval junc.occno=1
extract name="j2" xj material="Silicon"
  mat.occno=1  y.val=$yval junc.occno=2

extract name="arsenic" area from
  curve(depth,impurity="Arsenic"
  material="Silicon" mat.occno=1
  y.val=$yval) where x.min=$j1 and
  x.max=$j2 outfile="extract.dat"

set totalarsenic=($totalarsenic+
  ($arsenic*1e-4*$increment*1e-4
  *$width*1e-4))

extract name="boron" area from
  curve(depth,impurity="Boron"
  material="Silicon" mat.occno=1
  y.val=$yval) where x.min=$j1 and
  x.max=$j2 outfile="extract.dat"

set totalboron=($totalboron+
  ($boron*1e-4*$increment*1e-4
  *$width*1e-4))

set yval=($yval+$increment) L.END

# Print Final results
echo arsenic = $totalarsenic
echo boron = $totalboron

##################################################
```

The first seven lines use set statements that are used to assign values to variable names that will be used to define an approximate region of the device that will contain the well and to initialize variable values for the calculations.

Since we are calculating the number of species in the well volume, we have to specify the well dimension in the Z direction (into the screen). The "set width=1" line specifies the well is 1um into the Z direction. For different well dimensions, type in the appropriate length in microns here.

The "set depth=0.2" line will be used to specify that we want to integrate up to 0.2um into the depth of the silicon. As can be seen from figure 1, a depth of 0.2um is sufficient to accommodate the entire depth of the metallurgic boundary of the well. Once again, use an appropriate number for the depth of the well for your particular device. For the best accuracy and fastest calculation speed, use a depth that is only just deeper than the metallurgic junction of the well, so that the integration routine does not waste time looking for well regions that do not exist.

The "set steps=40" line will be used to instruct our integration routine to divide the integration region between Y=0 and Y=0.2um into 40 slices for the calculation. An optimum number of slices for your particular device would probably be something which creates slices which have approximately the same depth per slice as the smallest mesh spacing in the Y direction.

These three variables described above (width, depth and steps) can be modified by the user to suit their particular structure and level of required accuracy.

The next set of four variables, “increment”, “yval”, “totalarsenic” and “totalboron” initialize variables used in the calculations. The “increment”calculates how far to step down into the structure for each slice of the integration. Obviously, the increment value is the total depth of the integration, divided by the number of slices (steps).

The “yval” is the starting Y location for the first integration which is set to be in the middle of the first slice. “totalarsenic” and “totalboron” are the variables that store the accumulating totals for the number of boron and arsenic atoms that we are trying to calculate.

A “LOOP” statement as the name implies, will loop the section of the input file, bounded by the “L.END” statement, “step” times. In this example, we have requested 40 steps as this is the number of slices we are going to integrate.

The first two extract statements locate the first and second instances of the metallurgic junction in the horizontal direction for each slice. The third extract statement then integrates the number of arsenic atoms in the slice bounded by the metallurgic junctions by calculating the area under the concentration versus distance curve.

The following “set” statement then adds the total calculated arsenic atoms from each extracted slice, to the “totalarsenic” variable, so that after the final slice is integrated, it represents the total number of arsenic atoms in the whole well region. The total arsenic concentration will be in units of atoms/cm3, whereas all the distances over which we are integrating are in units of microns, so we have to multiply by 1e-4 in all three directions to get the correct number of atoms in the well region.

Each part of the loop described to integrate the number of arsenic atoms, is then repeated to calculate the number of boron atoms within the same loop. The “yval” variable at the end of the loop, is then increased by the “increment” value to define the depth of the next slice to be integrated. After the final slice is integrated, the “echo” statements simply asks DeckBuild to print out the values that it has calculated on completion.

In this particular example, the result of the integration was 2.96e7 arsenic atoms and 480,000 boron atoms, conforming to the expected result discussed at the begining of this article. The “missing” arsenic and boron atoms have diffused outside of the metallurgic boundary.

Conclusion

In conclusion, we have shown how to integrate the total number of any species in an arbitrary shaped well bounded by a metallurgic junction. This methodology can be adapted for other shaped wells and species of interest, such as calculating the number of electrons in an image sensor well at any time during the image capture process.

The Studies of Regular Texture Thickness and Finger Pattern of the Front Surface by Using Silvaco TCAD Tools

1. Introduction

The photovoltaic industry has rapidly grown since 2000 and has diversified in technology how the solar cell are manufactured. As of 2010, 70% of these cells were made from mono- and multicrystalline silicon wafer, 20% from thin films and 10% from silicon ribbons. In 1975, screen printing was first applied to solar cells for the formation of the front and rear contacts replacing expensive vacuum metallization [1]. This process and equipment for the screen-printed solar cell has been further optimized and new technologies have been introduced to improve this technology. These include an anti-reflection Silicon nitride coating with excellent surface and bulk passivity properties. Surface texture has reduced reflectivity. [2, 3] Laser edge isolation and single-side etching is used for the electrical separation of the front and rear contacts.

Silvaco TCAD [4] provides complete and well integrated simulation software for all solar cell technology. The TCAD modules required for solar cell simulation included: S-Pisces, Blaze, Luminous, Device 3D, and Luminous 3D.

In this article we will study a flat-type solar cell under different diffusion temperatures and concentrations. We will also study a texture-type solar cell with texture thickness and finger pattern at fixed shielding area of the front surface. We will find the maximum solar efficiency under different operation and design parameters.

2. Screen-Printed Silicon Solar Cell

Most screen-printed solar cells are fabricated in the industry today using the following process sequence: (1) Saw damage removal, texture and cleaning silicon wafer; (2) N-type diffusion; (3) Plasma edge isolation; (4) N-type glass removal; (5) Silicon nitride deposition; (6) Ag screen printing of the front contact and drying; (7) Al/Ag screen print of the rear busbars and drying; (8) Al screen printing of the backside contact and drying; (9) Conforming of the front and rear contacts; (10) Measure the IV curve.

3. Simulation of Solar Cell Characteristics Using Silvaco TCAD Tools

The parameters which we defined are listed in Table 1. Additional parameters used in simulation of solar cells, and its defaults, can be found in Silvaco TCAD manuals.

Parameter	Value	Unit
Cell Width	100	um
Cell Depth	200	um
Substrate Con. N-type	1e17	/cm3
Lifetime	10e-6	S
Light Source	AM15	-
Shielding area ratio	0.1	-
Workfunction For Al For Ag	 4.4 5.0	eV

Table 1. Parameters for Simulation.

3.1 Flat-type Solar Cell

(1) Diffusion concentration:
The simulation results are shown in Figure 1. We find that the Anode Voltage (Voc) increases along with the diffusion concentration is when the concentration is less than 5e+20. But we can also read from this figure that the Anode current (Isc) is almost the same at around -0.4.

(2) Diffusion temperature:
Figure 2 shows the simulation results with the diffusion temperature effect. We find that the Anode Voltage (Voc) increases with decreasing diffusion temperature. But we can read also from this figure that the Anode current (Isc) is almost the same at around -0.44.

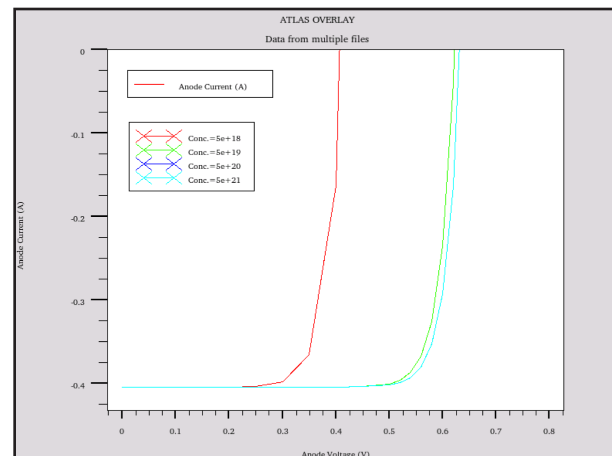


Figure 1. IV curve with diffusion concentration.

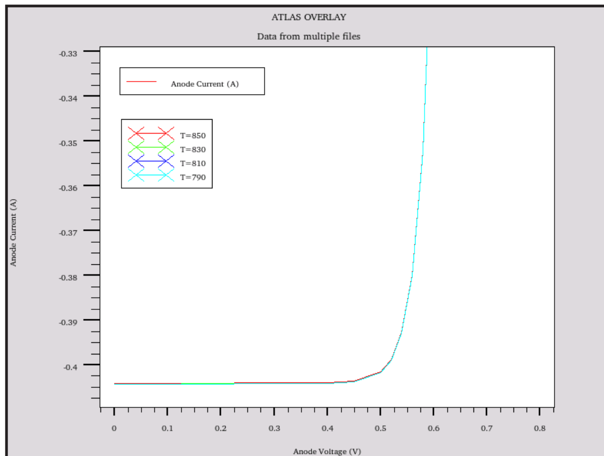


Figure 2. IV curve with diffusion temperature.

3.2 Texture-type Solar Cell

(1) Texture Thickness Effect:
The reflectivity and the IV curves of the simulation results are shown in Figures 3 and 4. From Figure 3 we can find that the reflectivity of the texture-type is smaller than that of the flat-type. The optimal condition, minimum reflectivity, for the texture thickness is 10um. Moreover, we also find that there is the maximum Anode Voltage value at texture thickness=10um.

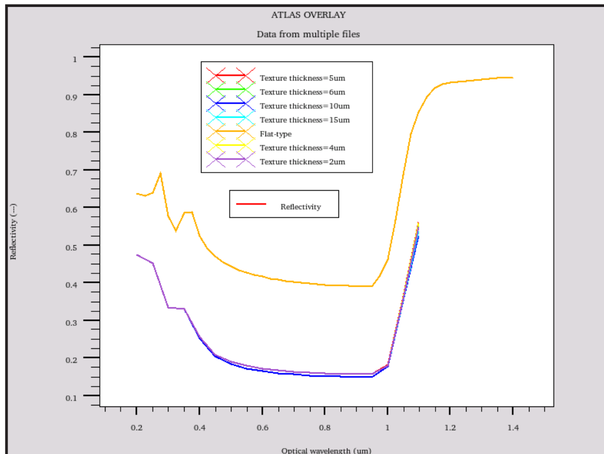


Figure 3. Reflectivity curve with texture thickness.

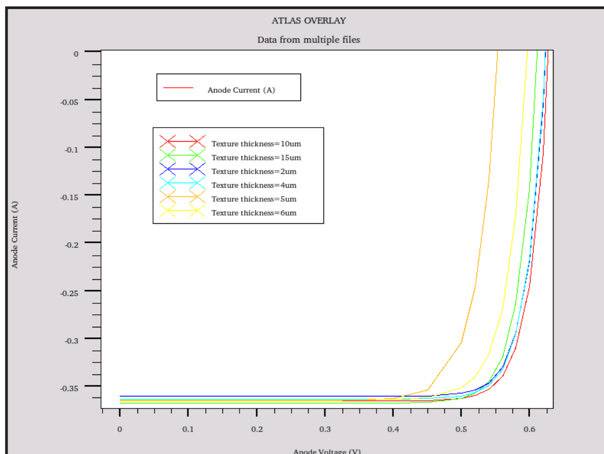


Figure 4. IV curve with texture thickness.

The summary of the solar cell efficiency is listed in Table 2. We find that the maximum efficiency at texture thickness equals to 10um.

Texture Thickness (um)	Efficiency (%)
2	15.45
4	15.56
5	13.17
10	15.77
15	15.40

Table 2. I Efficiency with Texture thickness.

(2) Finger Pattern under the Fixed Shielding Area:
According to the previous studies, we find that the optimal texture thickness is 10um, so we modified the finger pattern of the front surface under the shielding area so that the ratio equals 10%.

The pitch widths are 90um, 45um, 30 um and 15 um. The summary of the solar cell efficiency is listed in Table 3. We find that the maximum efficiency is where pitch width equals to 30um.

Pitch width (um)	Efficiency (%)
90	**15.77**
45	**13.16**
30	**16.24**
15	**12.37**

Table 3. Efficiency with Pitch Width.

4. Conclusion

In conclusion, Silvaco TCAD tool provides a complete solution for solar cell technology. In this article, it helps us to study the regular texture thickness and finger pattern of the front surface. We find the optimal design condition at texture thickness equals to 10um and the finger pitch width at 30um. It also enables researchers to study the all operation and design parameters of the Screen-Print Silicon Solar Cell.

Reference

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2. D. L. King and M. E. Buck, “Experimental optimization of an anisotropic etching process forrandom texturization of silicon solar cell,” Conference (PVSC ’91), vol. 1, pp. 303-308, Las Vegas, Nev, USA, October 1991.
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