Using VICTORY PROCESS for Rapid Geometry Prototyping Including Advanced Geometrical Operations

Introduction

The fully three-dimensional process simulator VICTORY PROCESS allows user to perform a wide range of manipulations of the structure's geometry in order to obtain the device of the desired shape. Most of the supported operations correspond to real technological processes (etching or deposition, CMP, epitaxy and others) so in many cases an engineer can establish a direct link between the technological processes step and an input deck statement of VICTORY PROCESS.

VICTORY PROCESS can simulate complicated full physics-based etching and deposition processes which take into account

- reactor characteristics (particle flux),
- shading effects and/or
- secondary effects like redeposition of the etched material

Naturally, such full physics-based simulations can take a long time and may be influenced by numerical error. However, many advanced operations may be performed very quickly and accurately using either the 'geometrical' mode of VICTORY PROCESS or very simple physical models. This paper covers several aspects of etching and deposition process characteristics which can be obtained by applying these fast operational modes of VICTORY PROCESS. Among those characteristics are :

- Rounded corners
- Tapered sidewall
- Non-conformal epitaxial growth
- Selective geometrical etch
- Selective CMP

In this paper we describe in details how each feature can be obtained.

Rounded Corners

The initial structure for this example is a silicon substrate covered by a thick layer of nitride. By etching geometrically with a mask and specifying the radius of the top corner:

```
SPECIFYMASKPOLY maskID=1   p="–1,–1" p="2,–1" \
                           p="2,0.5" p="–1,0.5"

GEOMETRYETCH thickness=0.38 maskID=1 reverse \
          cornerRadius=0.02
```

you obtain the structure as shown in Figure 1a). The pattern described by the mask layer with the identification number 1 (the shape of this mask layer is defined by the SPECIFYMASKPOLY statement) is transferred into the nitride layer. The top corner of the transferred pattern is rounded with a corner radius of 20nm as determined by the cornerRadius option of the GEOMETRYETCH statement. For illustration purposes Figure 1b) shows the structure obtained by the same etching statement, but without setting the corner radius. In this case the resulting top corner of the transferred pattern is sharp. It is worth mentioning that in this example several technological steps (depositing the resist, etching the exposed nitride, removing the resist layer and, possibly, corner rounding) were simulated by a single simulator input deck statement.
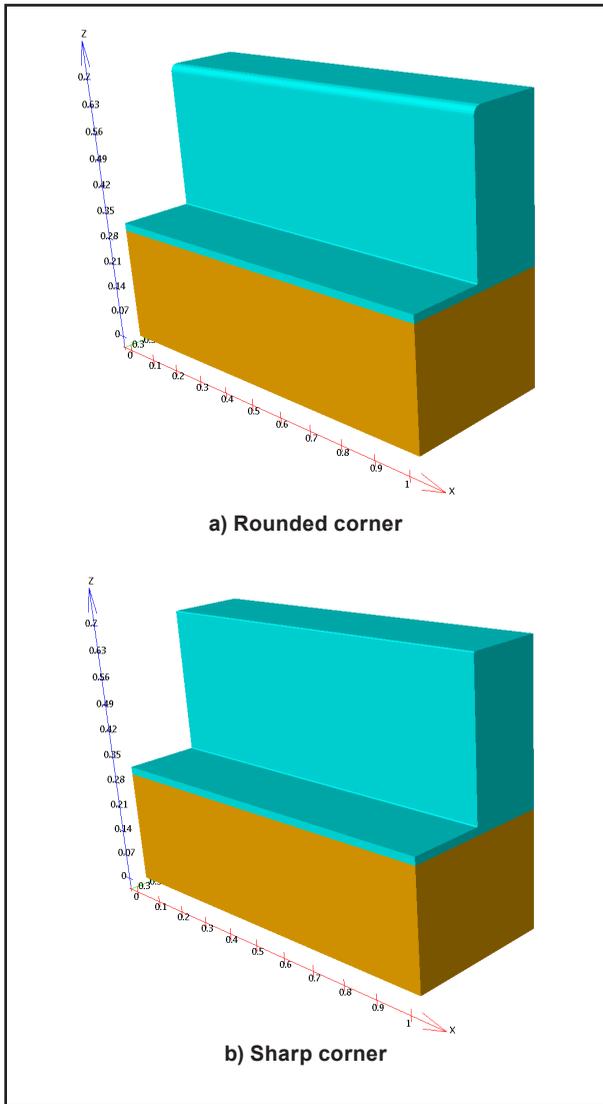
a) Rounded corner

b) Sharp corner

Figure 1. Etching with automatic corner rounding.

Planar Deposition

Sometimes it is necessary to fill the trench or cavity in the structure with a certain material up to a given level. VICTORY PROCESS allows to do it with a single input deck statement using the planar deposition mode.

Continuing from the structure shown in Figure 1a) you may grow two pillars of different materials through the thin layer of nitride. You can achieve this by etching two holes down to the surface of silicon and then vertically depositing, say silicon and polysilicon over those holes. To do this you can apply the following sequence of statements :

```
SPECIFYMASKPOLY maskID=2        p="0.20,-1"  \
                                p="0.35,-1"  \
                                p="0.35,0.5" \
                                p="0.20,0.5"
SPECIFYMASKPOLY maskID=3        p="0.65,-1"  \
                                p="0.80,-1"  \
                                p="0.80,0.5" \
                                p="0.65,0.5" \
```

```
GEOMETRYETCH thickness=0.02 maskID=2 reverse
GEOMETRYETCH thickness=0.02 maskID=3 reverse
GEOMETRYDEPO thickness=0.20 maskID=2 \
             material=silicon directional=on
GEOMETRYDEPO thickness=0.20 maskID=3
             material=poly directional=on
```

The resulting structure is shown in Figure 2a). The next step could be to cover the thin layer of nitride with the thin layer of aluminum. Because several different masks were used to etch the nitride and grow the pillars, it is not straightforward to obtain the necessary structure using ordinary directional deposition. One solution would be to use selective deposition with a mask (deposit the aluminum selectively over the nitride only, with the mask with identification number 1 used in the previous section). However, this requires invoking a physics-based model, which takes considerably more time to run than geometrical operations. With planar deposition we can obtain the required shape very fast, with high degree of numerical accuracy and using a single statement :
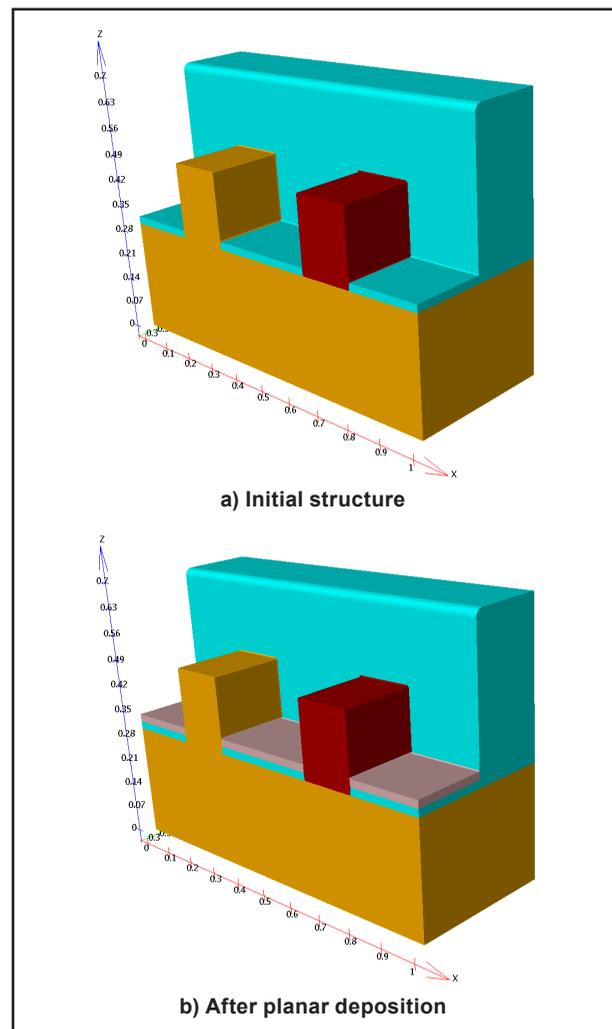
```
GEOMETRYDEPO material=aluminum planar z=0.34
```


a) Initial structure

b) After planar deposition

Figure 2. Planar deposition example.

Here parameter z specifies the vertical coordinate up to which the structure should be filled. The identical structure could be obtained by specifying the relative distance from the highest point of the structure via parameter fromTop."

```
GEOMETRYDEPO material=aluminum planar \
                fromTop=-0.36
```

The result is shown in Figure 2b).

Epitaxy

One important process in semiconductor industry is epitaxial growth. With selective deposition you can emulate both conformal and non-conformal epitaxial growth over 3D structures in a rather simple manner.

Starting from the structure shown in Figure 2b) of the previous section you may want to grow silicon non-conformally over the silicon pillar. To do so a selective physics-based deposition model can be applied. To illustrate how to grow one material over another, we shall grow the silicon over the polysilicon pillar as well. First you have to define:

- the rate   - speed of growth over horizontal surfaces and

- the ratio   - how much the growth over vertical walls is slower

with the following statement:

```
ETCHDEPOPROPERTIES name=epitaxy \
    material=silicon rate=0.075 ratio=0.5 \
    material=poly    rate=0.075 ratio=0.5
```

Note, that this statement defines material *over* which growth will occur, not which material will be *grown*. The next statement performs the actual deposition using the properties defined above.

```
DEPOSIT material=silicon \
        materialproperties=epitaxy \
        time=1.0 model=nonconformal \
        maxCFL=1
```

The resulting shape is shown in Figure 3a).

Note, that although in statement ETCHDEPOPROPERTIES we could, for example, set rate and ratio for growth over polysilicon different from those for silicon, it would not significantly change the results. The reason for this is that after the first time step all exposed polysilicon will be covered with silicon and the process will continue using the silicon's rates. An important consequence of this is that you must include the deposited material in the list of material in the ETCHDEPOPROPERTIES statement, otherwise the growth will be stopped after the first time step. Figure 3b) shows

a) Silicon was grown over silicon and polysilicon

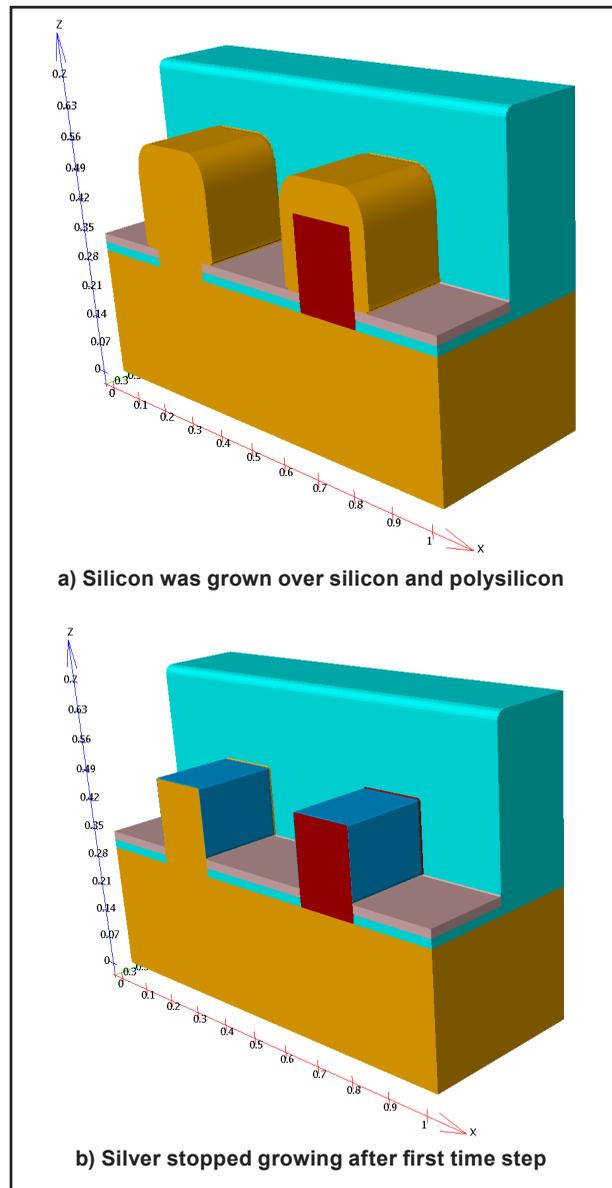**b) Silver stopped growing after first time step**

Figure 3. Epitaxial growth example.

the results of an attempt to grow silver instead of silicon using the same material properties as defined above :

```
DEPOSIT material=silver \
        materialproperties=epitaxy \
        time=1.0 model=nonconformal \
        maxCFL=1
```

As the default rate for growth over materials, which are undefined in the statement ETCHDEPOPROPERTIES, is zero, once silver covered all exposed silicon and polysilicon no further growth does occur.

Finally, note, that although seemingly simple, the selective growth is highly non-linear process due to the step change in growth rates over different materials, therefore, careful adjustment of the deposition time step is required. If the sim-

ulation is done with more than one level of geometrical mesh refinement we suggest always to set the option `maxCFL=1` in the `DEPOSIT` statement which imposes stronger conditions on the time step control than the default set-up.

Tapered Sidewall

The following example illustrates how one can obtain a tapered side wall using geometrical etching.

Starting from the structure shown in Figure 3a) you may want to fill it with oxide up to the top of the silicon pillars and with a slope from the middle of the pillars to the top of the nitride. The easiest way to obtain this shape is by first filling the structure to the top with oxide using planar deposition and then etching with a mask and specifying a sidewall angle (`angle=38.66`) for the etching process :

```
GEOMETRYDEPO material=oxide planar fromTop=0
GEOMETRYETCH maskID=1 thickness=0.125 dry \
             angle=38.66 reverse
```

Figure 4a) shows the resulting structure. The value assigned to the angle option was obtained by the following calculations:

The distance from the top of the silicon pillar to the top of nitride is 0.125μm, the half width of the pillars (along Y axis) is 0.1μm. Therefore the required angle is $\tan^{-1}(0.1/0.125)$=38.66 degrees. Note, that the same mask was used as in the first section of this paper, to ensure the correct position of the corner.

While on Figure 4a) the tapered sidewall reaches the top of the nitride step, you might want it to start just below the rounded corner instead. This can be achieved by changing the parameters of `GEOMETRYETCH` statement in the following manner :

```
GEOMETRYETCH maskID=1 thickness=0.125 dry \
angle=43.60 reverse \
             deltaCD=0.019 material=oxide
```

Notice the required changes:

- The angle now is different, as the slope now should reach the height 0.02 below the top of the nitride step, but its width did not change, hence its angle now is $\tan^{-1}(0.1/1.105)$=43.60 degrees

- If continued through the nitride to the top, the slope would end at $\tan(46.47)0.02$=0.019μm from the nitride step's edge, therefore we need to use the option `deltaCD=0.019`, which shifts the mask edge by 19 nm

- Finally, we now have to use selective etching (see next section) to etch oxide only, otherwise the nitride corner will be 'shaved off' to continue the slope
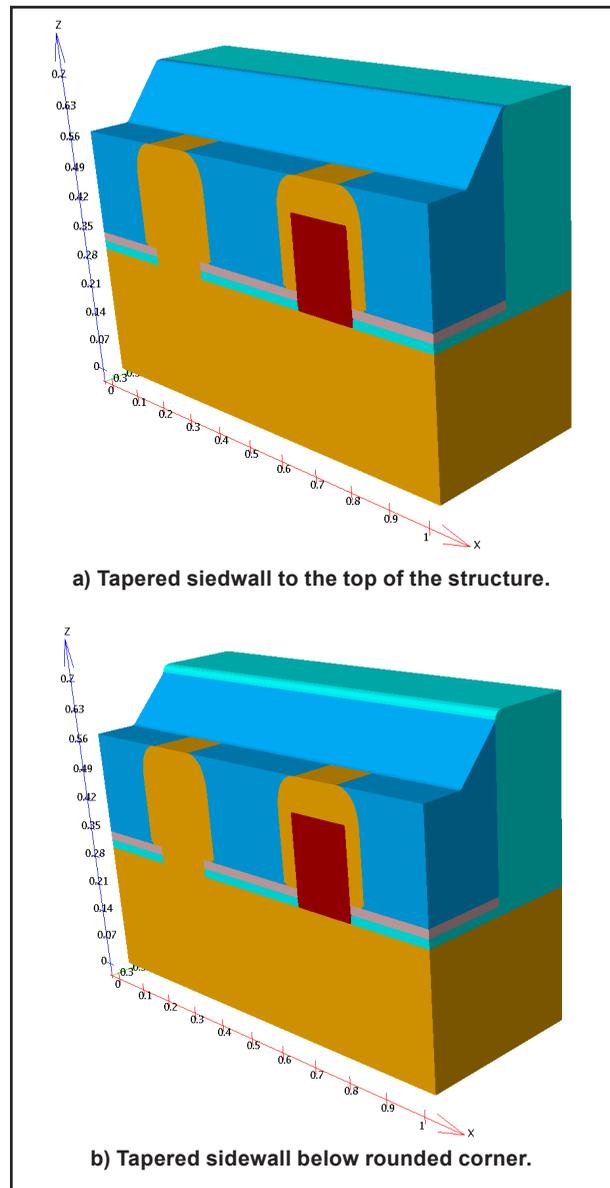
The resulting structure is shown on Figure 4b).

a) Tapered siedwall to the top of the structure.

b) Tapered sidewall below rounded corner.

Figure 4. Tapered corner example.

Selective Etch and CMP

As it became apparent from the previous sections, it is sometimes necessary to remove a particular material only. This can be achieved by means of physical-based selective etching, but this approach has the same implications as mentioned in the above section dealing with physical deposition. Alternatively, VICTORY PROCESS allows you to remove material selectively also in the geometrical mode using either `GEOMETRYETCH` or `GEOMETRYCMP` statements.

For instance, you may want to remove the planar part of the oxide step in the structure in Figure 4b) down to aluminum. We know, that it starts half way from the silicon pillar's width which is 0.1 μm from the nitride step's edge. Therefore we need to etch oxide only, stepping

away 0.1 *μ*m from the edge of the nitride. For that purpose you can again use the mask with the identification number 1 as defined in the first section of this paper and offset the mask edge by means of the `deltaCD` option of the `GEOMETRYETCH` statement :

```
GEOMETRYETCH thickness=0.235 maskID=1 \
             deltaCD=-0.1 reverse \
             material=oxide
```

The result of this etching process is shown on Figure 5a).

The effect of selective CMP is reverse to planar deposition. In case of selective CMP the given material is removed from the structure up to the specified position (which is set either as a distance from the highest point of the structure or as an explicit z-coordinate). The statement

```
GEOMETRYCMP thickness=0.0625 material=oxide
```

removes the tapered oxide sidewall halfway between top of the structure and the top of the silicon pillar. The resulting structure is shown on Figure 5b).

Conclusion

VICTORY PROCESS is capable of performing the wide range of geometrical manipulations of the structure, with many operations corresponding to the real technological processes. In many cases the desired results (e.g. rounded corners or tapered sidewalls) may be achieved using the numerically highly accurate and fast geometrical mode, which does not involve modeling of the real physical processes. The 'physics-based' mode can be used to simulate conformal or non-conformal epitaxial growth over complicated 3D topography.
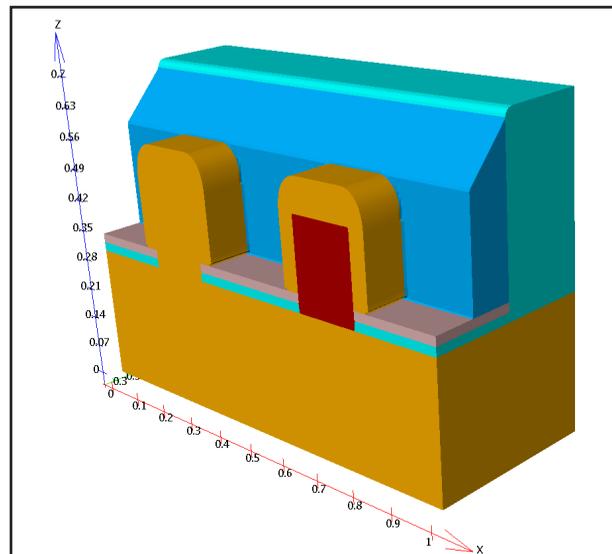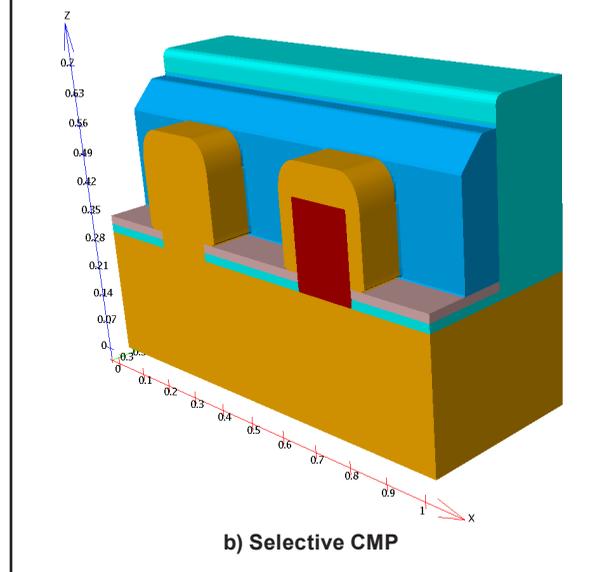

Figure 5. Selective material removal

b) Selective CMP

Figure 5. Selective material removal.