SYSC 5104
Discrete – Event Modeling and Simulation

Assignment 2: Si Atom Etching Process Simulation using Cell-DEVS

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1. Introduction

Etching is the process of using strong acid or other methods to cut into the unprotected part of a material. In semiconductor manufacture industry, the etching of silicon is widely and frequently used. For example, MEMS (Micro Electro Mechanical Systems), a new technology, which is combined with microelectronics and mechanical engineering, uses etching technique to fabricate different kinds of structures on the surface of silicon wafers. Those structures could be cantilever beam which is part of a new kind of resonator, or even vibrating structure used for MEMS gyroscope.

Etching techniques could be classified into two major categories: wet etching and dry etching. The major difference between them is that the wet etching uses solution or solvent to etch the target material. Considering the manufacturing and testing of a structure or circuit on the wafer will cost a lot of money and time, and there is also a great possibility of failure, fine designed simulation is strongly needed. This kind of simulations will help to reduce the research cost and shorten research cycle.

In our simulation, we apply cell-DEVS into simulating Si wet etching process. Wet etching is the process of using chemical reaction between some special liquid and wafer to remove the part uncovered by the photoresist. As wet etching is a pure chemical process, it has advanced selectivity which stops at current thin-film without affecting other material.

In Si wet etching, the etching speed appears to be different with different crystal planes. Specifically speaking, (111) plane density is larger than the (100) plane, so the etching speed of (111) plane will be lower than that of (100) plane. In application, if the Si on (100) plane is covered by SiO_2 with certain pattern, the directional etchant will generate an accurate V slot with border being (111) plane and angle being 54.7 degree with (100) plane, as showed in Figure 1-1.

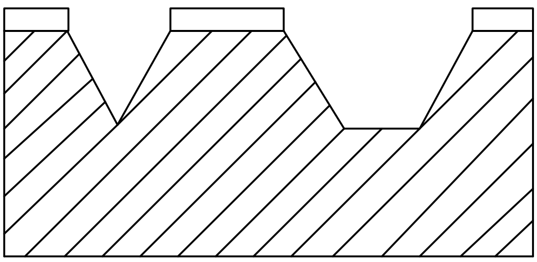


Figure 1-1 V slot of (100) plane and (111) plane

Our simulation is to reproduce the whole process of forming V slot in Cell-DEVS. Cell-DEVS is a formalism used to simulate the complex physical model into cell space model, which is required to be time discrete, space discrete and state discrete. Considering from the Si stereochemical structure, each Si atom can be seen as a cell and they are distributed discretely in Si molecule. For detailed illustration of Si etching process with Cell-DEVS, we describe in the following.

2. 3D Model Specification

2.1 Conceptual Model

Before etching process, we should understand the basic information about Si atom structure. Actually, Si atom can connect with each other in covalent bond, as showed in Figure 2-1. Wafer is composed of a large number of such Si atom and connected with covalent bond. On the base of basic Si atom structure, we can divide wafer into many layers with four different layers as a cycle, others are just repeat such four layers.

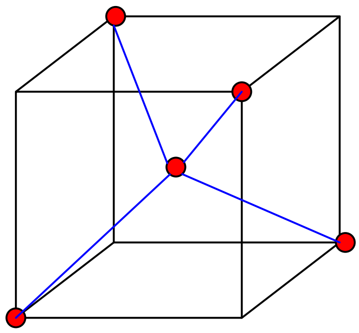
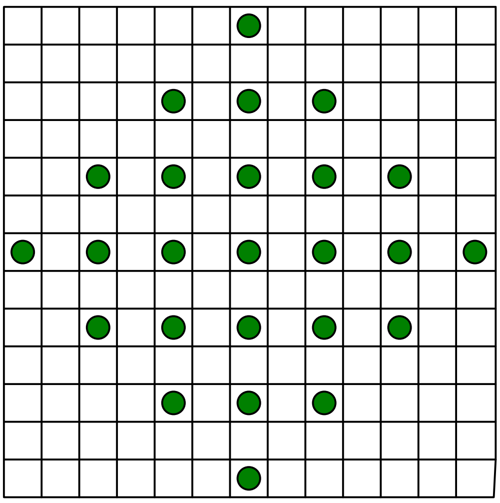
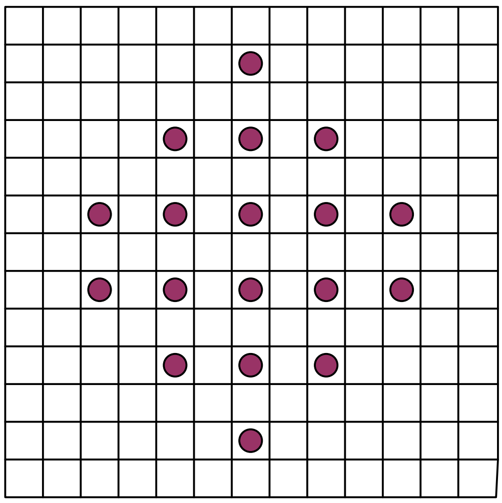


Figure 2-1 Si atom structure

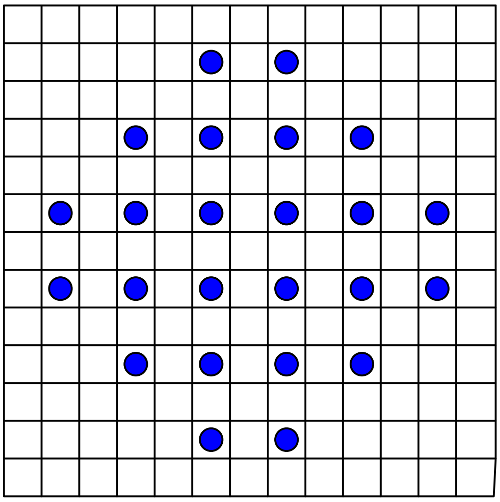
Follows are the platform of layers of atoms, in the substrate, each unit cell of silicon can be divided in 5 layers, and we repeat every 4 layers, when arranged in periodic lattice. That means, the first layer has the same platform with the fifth layer. The specific layers are indicated as follows:



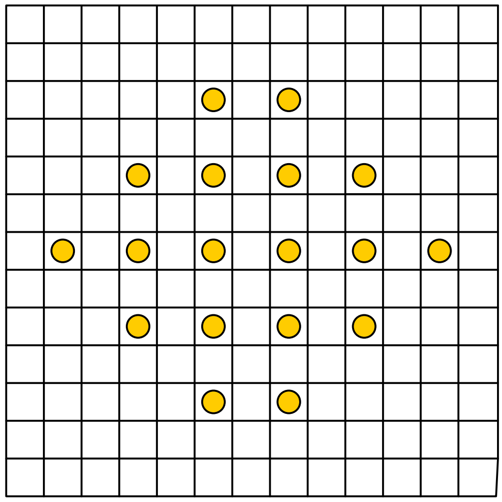
Layer 1



Layer 2



Layer 3



Layer 4

As we only highlight some atoms in each layer to see their difference, the actual model is that Si atoms are distributed in the whole plane. Observing the above figures, we know that layer 2 is layer 1 translating a line downward, layer 3 is layer 1 translating a line downward and translating a column to the right, while the layer 4 is layer 1 translating a column to the right. These platforms are correspond to [110] direction, and [100] direction could be seen after rotating these platforms for 45◦. And we also assume that in lateral dimensions the atom layers are infinite. Each atom has four bonds, each one of the bonds may have two different states, one is complete and the other one is incomplete. And we could regard the atoms at the other side of the bonds as the neighbors of this atom. Incomplete bond means there are no atoms connect to this atom and complete bond means the opposite.

According to the wet etching feature, we defined the atom three states:
0 – Removed; this atom will be etched.
1 – Keep; this atom won't be etched.
2 – Surface; this atom is the surface atom.

Their operating rules are defined as:
1. If a cell (atom) is in Keep state and have two complete bonds and two incomplete bonds, the next state of the cell (atom) is Removed;
2. If a cell (atom) is in Keep state and have less than four complete bonds, this cell (atom) is Surface atom.
3. (a) If a cell (atom) is in Keep state and have three complete bonds, and at least one bond is with surface atoms, then the next state is Removed;
(b) If a cell (atom) is in Keep state and have three complete bonds, all with substrate atoms, the next state is Keep;
4. If a cell (atom) is in Keep state and have four complete bonds, the next state is Keep;
5. If an atom does not agree with any of the above rules, then its next state is Removed.

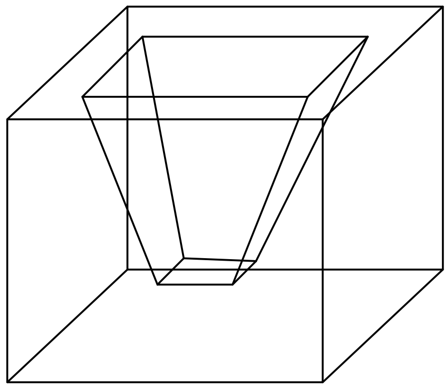


Figure 2-3 Etching finish plan

Following the rules defined above, the finished etching chart should be as Figure 2-3 shows. In the final, atoms in (100) plain should be etched, as described in rule 1; atoms in (110) plain should be etched too, as described in rule 3(a); atoms in (111) plain should be kept, as described in rule 3(b). Figure 2-3 is the 3D visualization, which we will show in the attended video, but the result analysis is illustrated in 2D view for simple.

2.2 Cell-DEVS Formal Specifications

As Si structure is complex with four covalent bonds each Si atom, we consider is as a cube as simple. Showed in Figure 2-4, the central black cube is the considering cell, and it has 27 neighbors in total. During the etching process, all its neighbors' states should be put into consideration.

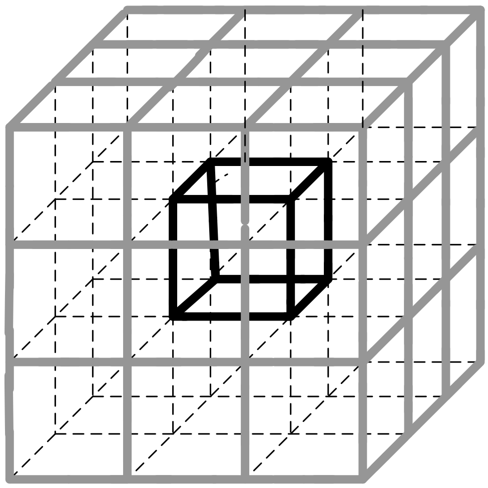


Figure 2-4 Si cell neighbor structure

So, the Cell_DEVS formal specification can be written as:

$$CD = \langle X, Y, I, S, \theta, N, D, \delta_{int}, \delta_{ext}, \tau, \lambda, D \rangle$$

Where

$X = \phi$,

$Y = \phi$,

$I = \langle \eta, P^x, P^y \rangle$,

where η= 27,

P^x = { all in neighborhood },

P^y = { all in neighborhood },

S = { 0, 1, 2 },

// 0: Removed

// 1: Keep

// 2: Surface

Θ = { (s, phase, f, σ), s ϵ S = { 0, 1, 2 }, phase ϵ {active, passive}, σ = 100 },

N = { (-1, -1 ,1)   (-1, 0, 1)   (-1, 1, 1)
(0, -1, 1)   (0, 0, 1)   (0, 1, 1)
(1, -1, 1)   (1, 0, 1)   (1, 1, 1)
(-1, -1, 0)   (-1, 0, 0)   (-1, 1, 0)
(0, -1, 0)   (0, 0, 0)   (0, 1, 0)
(1, -1, 0)   (1, 0, 0)   (1, 1, 0)
(-1, -1, -1)   (-1, 0, -1)   (-1, 1, -1)
(0, -1, -1)   (0, 0, -1)   (0, 1, -1)
(1, -1, -1)   (1, 0, -1)   (1, 1, -1) },

D = transport delay 100ms,

δ_{int} = { rule1 : if (0,0,0) = 1 and truecount < 5, next state is 2 after 100ms,

rule2 : if(0,0,0) = 2 and statecount(0) = 24, next state is 0 after 100ms,

rule3 : if (0,0,0) = 2 and statecount(0) = 23 and statecount(2) >= 2, next state is 0 after 100ms

rule4 : if (0,0,0) = 2 and statecount(0) = 23 and statecount(2) = 0, next state is 1 after 100ms,

rule5 : if (0,0,0) = 2, next state is 1 ater100 ms,

rule6 : if(0,0,0 next state is) = 1 and truecount = 5, next state is 1 after 100ms,

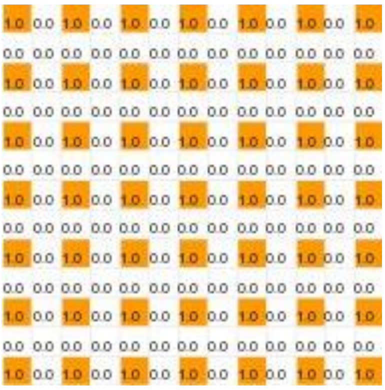
rule7 : if else, next state is 0 after 100 ms, }

δ_{ext} = ϕ,

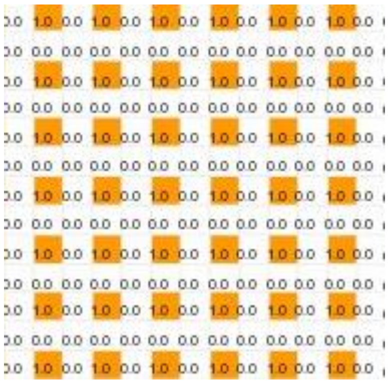
3. Result and Analysis

As the following shows, the Si atoms in each layer varies with the time elapsed. The time interval is set to be 100ms, so we illustrate the result in sequence of time. Here, for simplicity, we consider 13×13 cells in each layer with 8 layers in total. As four layers is a repeat cycle, the atoms distribution only has four possibilities. In simulation, we use 1 representing Keep state, 0 representing Removed state and 2 representing Surface atom. As the screen cannot display all layers, we pasta the first 6 layers here to observe the change.

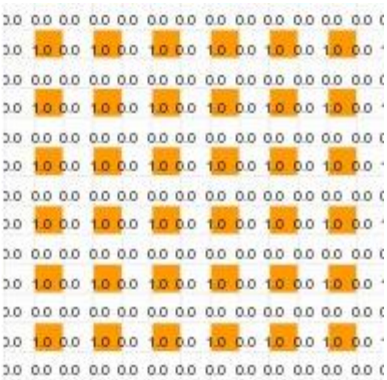
Time = 00:00:00:000



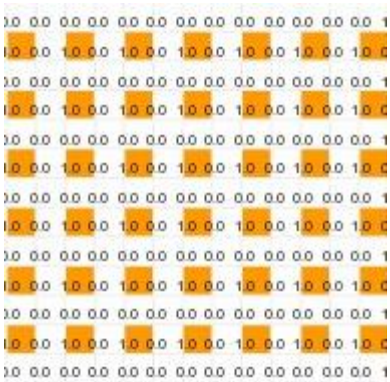
Layer 1



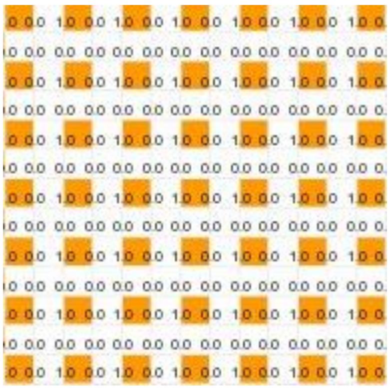
Layer 2



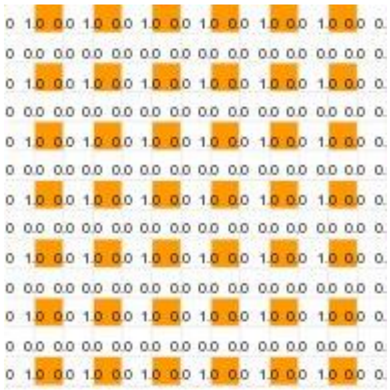
Layer 3



Layer 4



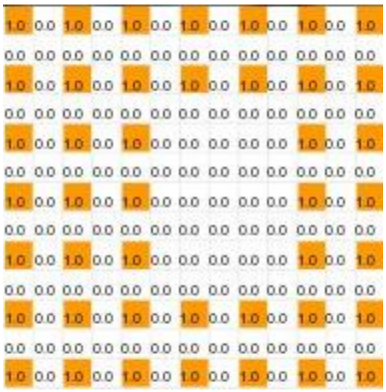
Layer 5



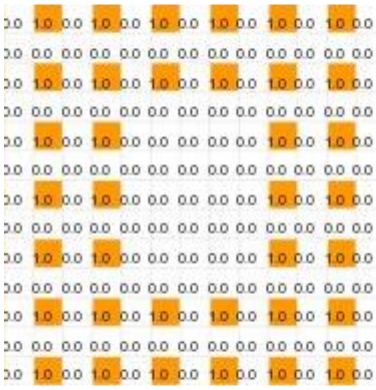
Layer 6

This is the initial state of Si atoms before etching process, and the atom place is as defined in Specification. It is worth noting that the state and distribution of atoms in Layer 5 and 6 are the same as that in Layer 1 and 2. That is because Si structure can be separated in four different layers with others being kept repeated.

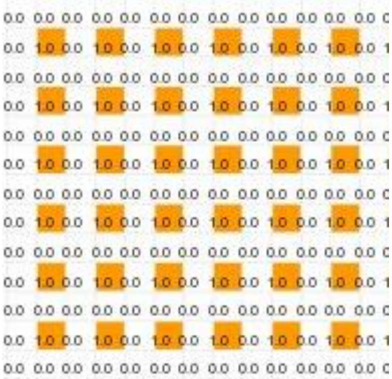
Time = 00:00:00:100



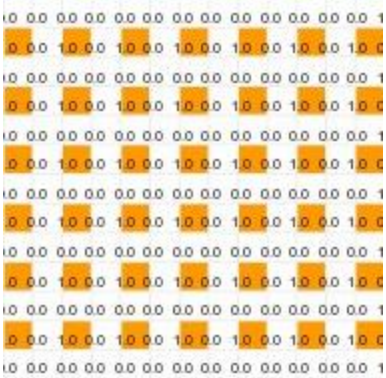
Layer 1



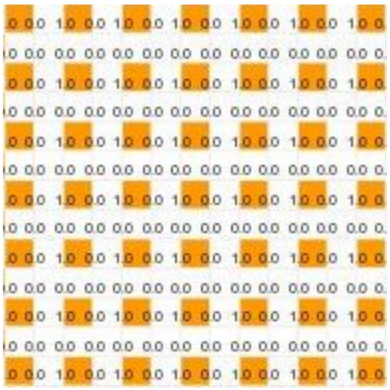
Layer 2



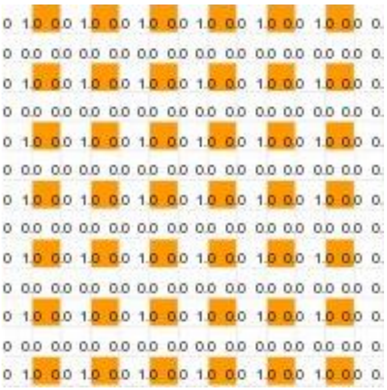
Layer 3



Layer 4



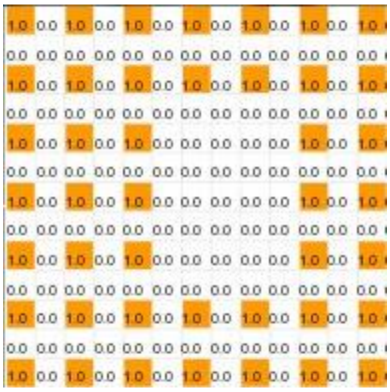
Layer 5



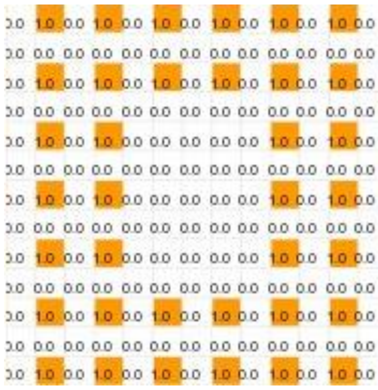
Layer 6

When compared with the figure in Time = 00:00:00:000, the atoms in layer 1 and 2 here change. Following the rule defined before: If a cell (atom) is in Keep state and have two complete bonds and two incomplete bonds, the next state of the cell (atom) is Removed; the atoms of state 1 in the middle are etched, while the surroundings are kept remained because of mask protection.

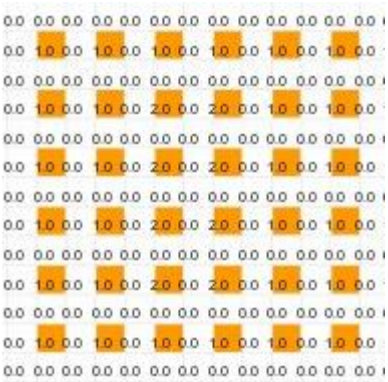
Time = 00:00:00:200



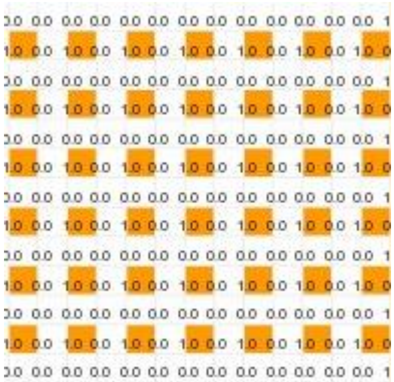
Layer 1



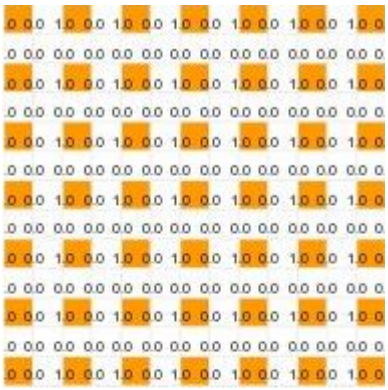
Layer 2



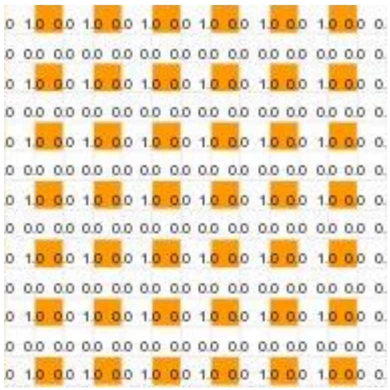
Layer 3



Layer 4



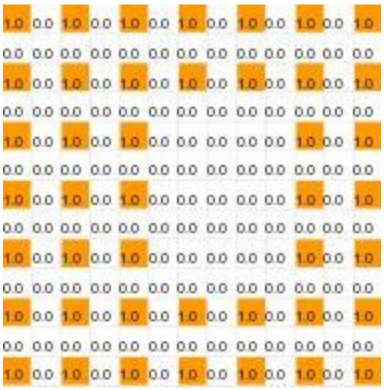
Layer 5



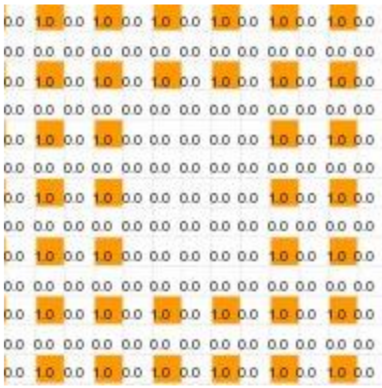
Layer 6

Comparing with the last time interval, some atoms in layer 3 change the sate of 1 to 2, indicating that they are the surface atoms. As rule defined: If a cell (atom) is in Keep state and have less than four complete bonds, this cell (atom) is Surface atom. The atoms changed here because some atoms in layer 2 have already been etched, they don't have enough four bonds.

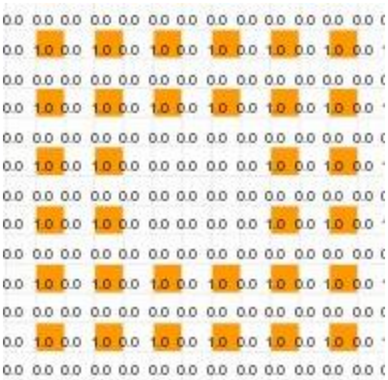
Time = 00:00:00:300



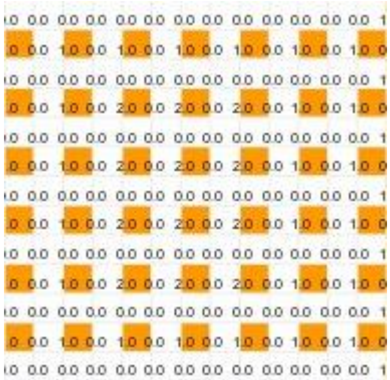
Layer 1



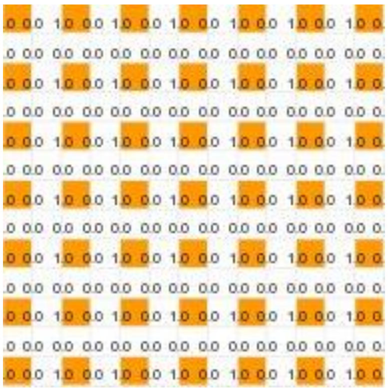
Layer 2



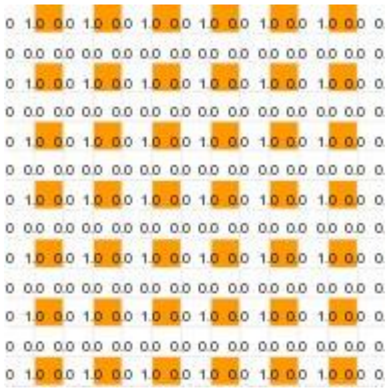
Layer 3



Layer 4



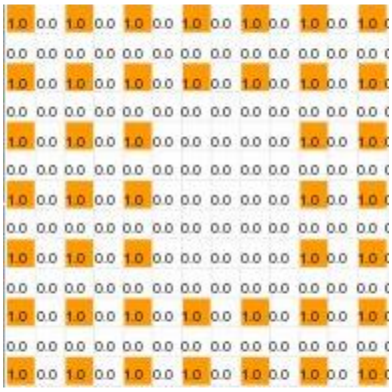
Layer 5



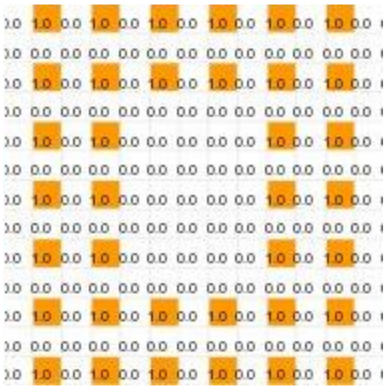
Layer 6

Similar to the above, layer 3 finishes etching and Layer 4 changes state. As defined: If a cell (atom) is in Keep state and have three complete bonds, it will become Removed when at least one bond is with Surface atoms, or Keep when all bonds with substrate atoms. In such case, some atoms in the layer 3, at least one bond is with Surface atoms, are etched. Similar to the Time = 00:00:00:200, some atoms in the layer 4 change their state.

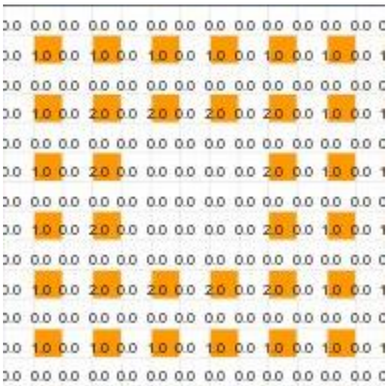
Time = 00:00:00:400



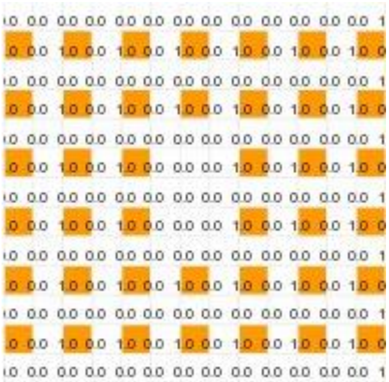
Layer 1



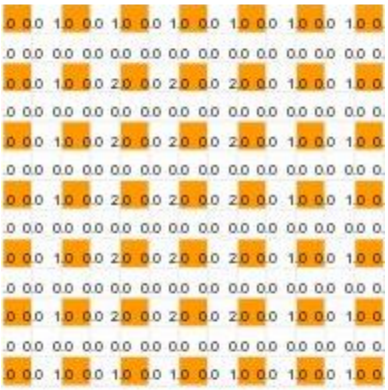
Layer 2



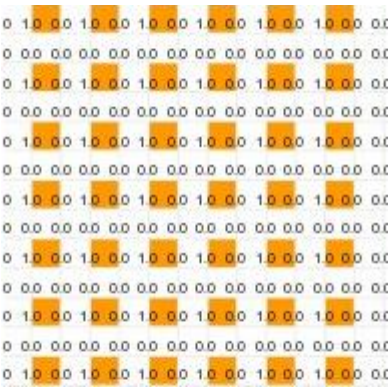
Layer 3



Layer 4



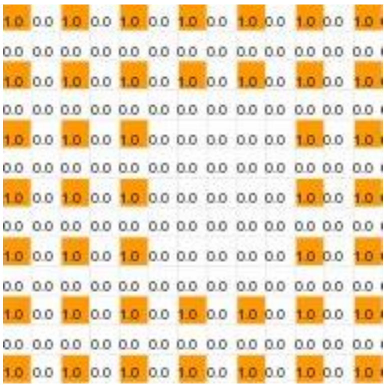
Layer 5



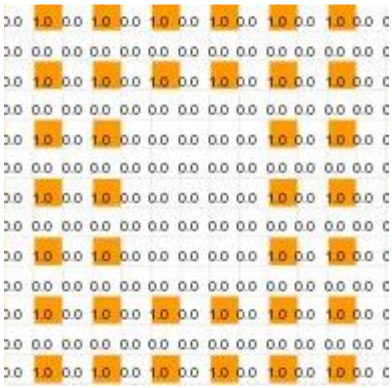
Layer 6

It's clearly to see that the layer 4 has been etched too while the layer 5 changes state. It is worth noting that the etching process won't affect the layers have already been processed.

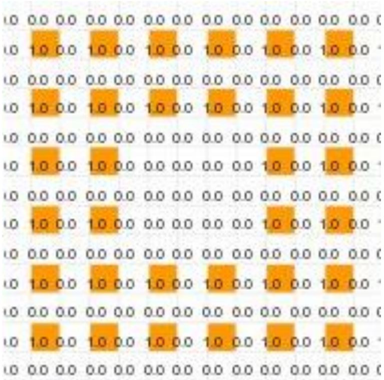
Time = 00:00:00:500



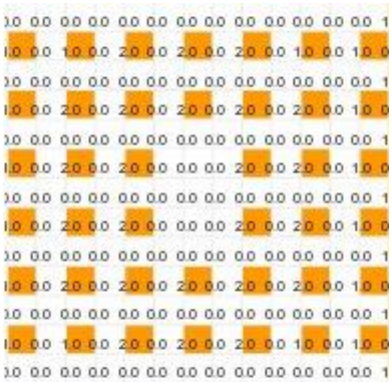
Layer 1



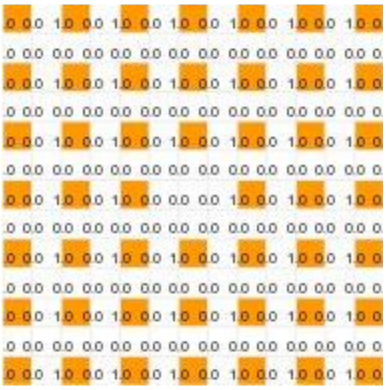
Layer 2



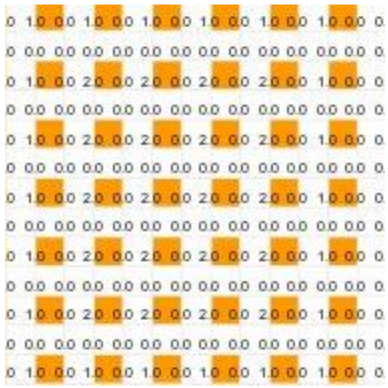
Layer 3



Layer 4



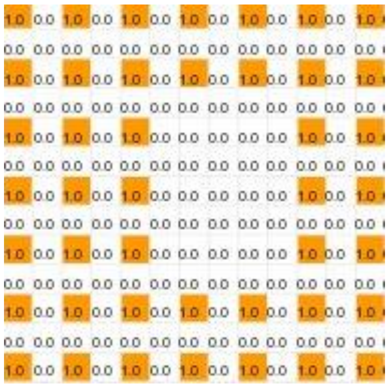
Layer 5



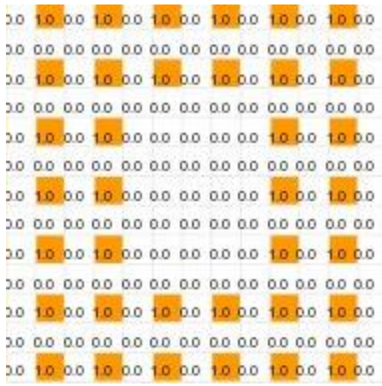
Layer 6

After another 100ms, the etching process keeps going deeper. At the Time = 00:00:00:500, atoms in layer 5 are etched but the state changing happens in both layer 4 and layer 6. That is because each time applying the rules defined, it will scan all layers from top to the bottom. As defined, the atom changes its state to 2 when it has less than four bonds, so layer 4 also convert the state of atoms satisfying condition.

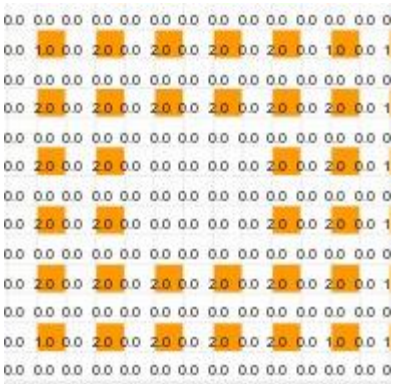
Time = 00:00:00:600



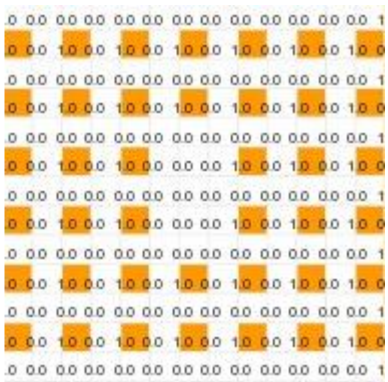
Layer 1



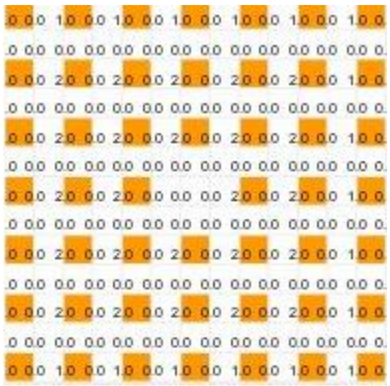
Layer 2



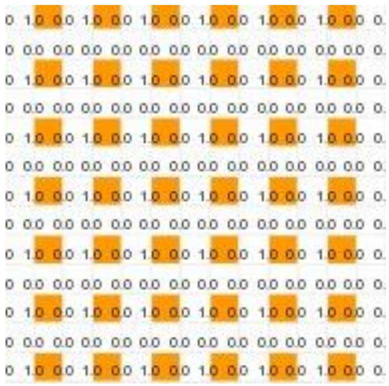
Layer 3



Layer 4



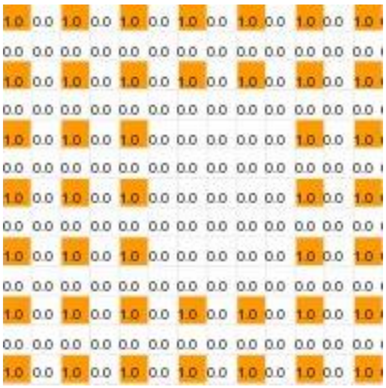
Layer 5



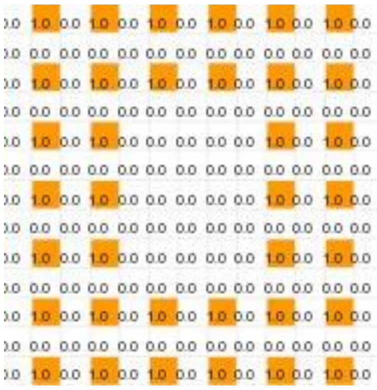
Layer 6

For simplicity, we use 13*13*8 dimension and set that only etching first 5 layers. In such case, the etching process can be said as finished, because layer 5 has already been etched successfully. But other atoms will continue to change their state for the rest time. To illustrate clearly, we capture another time interval to observe the state change below.

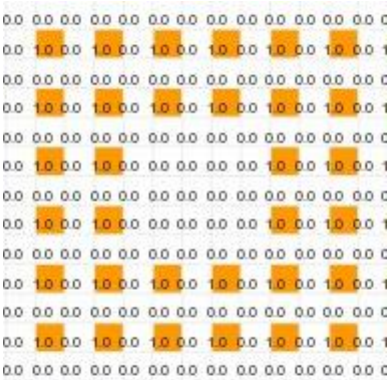
Time = 00:00:00:700



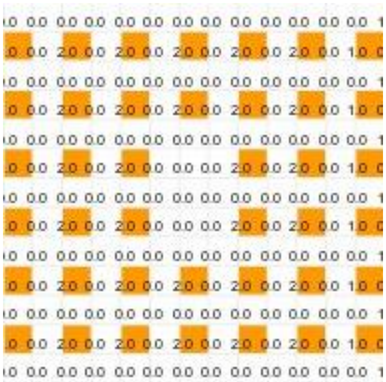
Layer 1



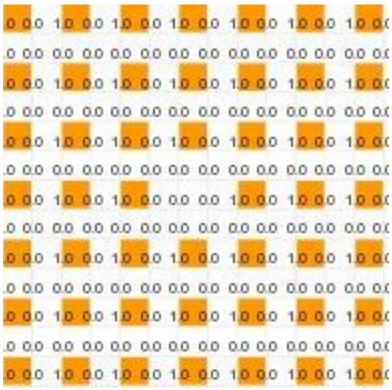
Layer 2



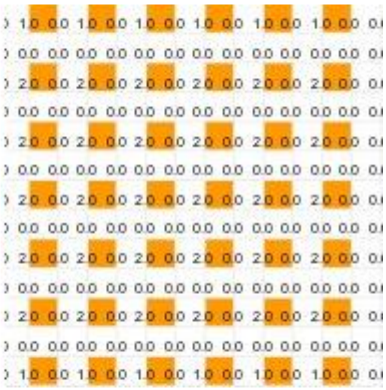
Layer 3



Layer 4



Layer 5



Layer 6

Now, the state change again but the etching has finished. From the above figures we can observe the whole etching process step by step following the rules defined and the result is as our expected before. So, our Si etching cellular automata simulation is successful and correct.

To make our simulation model more convectively, we expand the cell number and layer number to 30*30*9, which can, to a large extend, avoid the problems caused by small number of structure. In addition, we etch a different pattern – cantilever. The values verified are cell size and zone:

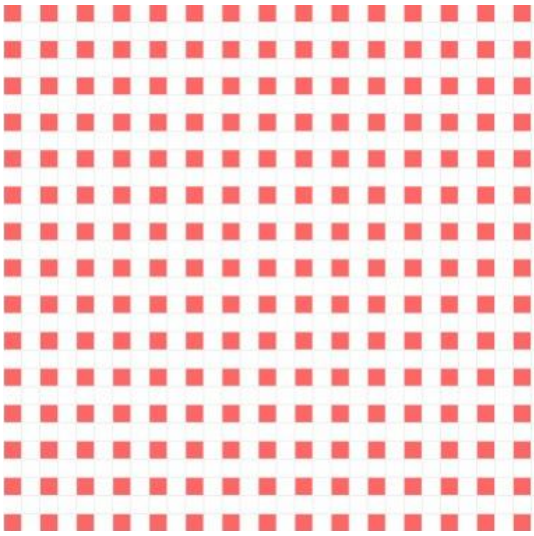
zone : etching-rule { (1,1,1)..(27,27,8) }

zone : surface { (1,1,0)..(27,4,0) (1,15,0)..(27,27,0) }

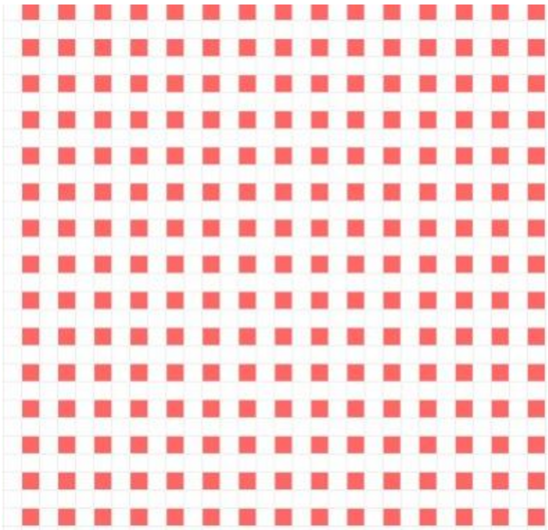
zone : mask { (1,5,0)..(27,14,0) (0,0,0)..(29,0,8) (0,0,0)..(0,29,8)
(28,1,0)..(29,29,8) (1,28,0)..(29,29,8) }

As following shows, we can observe the cantilever clearly and obviously. As the screen cannot display all layers, we only pasta the first three layers here to observe the change trend.

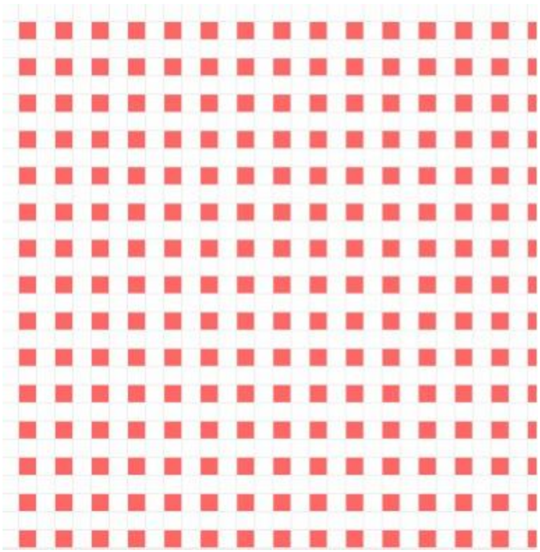
Time = 00:00:00:000



Layer 1

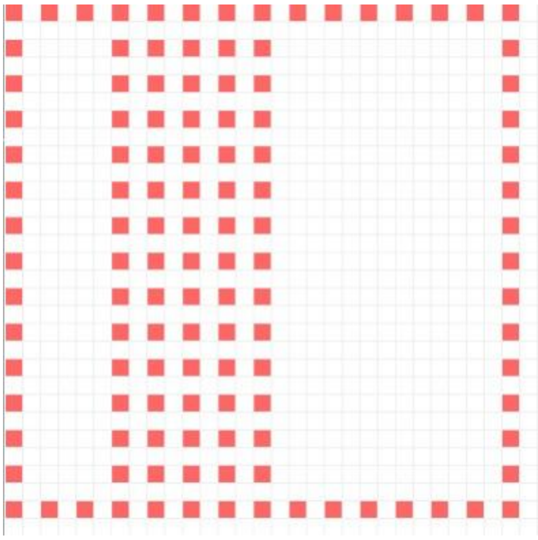


Layer 2

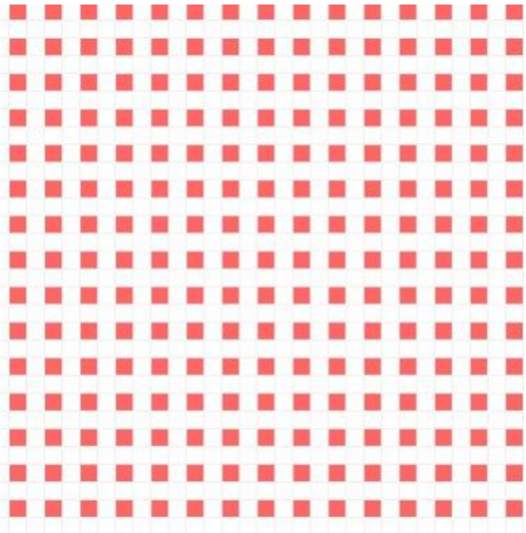


Layer 3

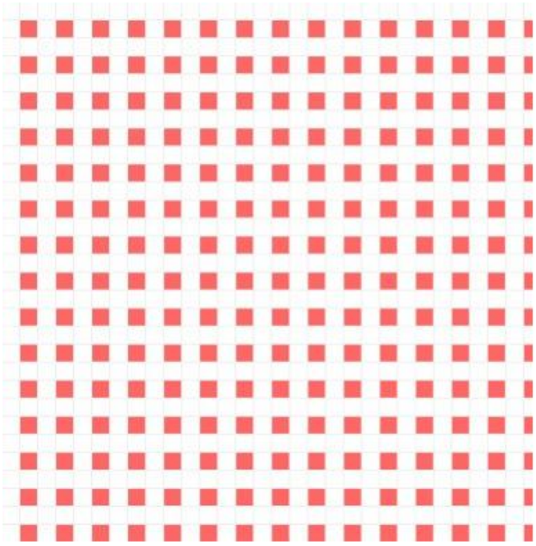
Time = 00:00:00:100



Layer 1

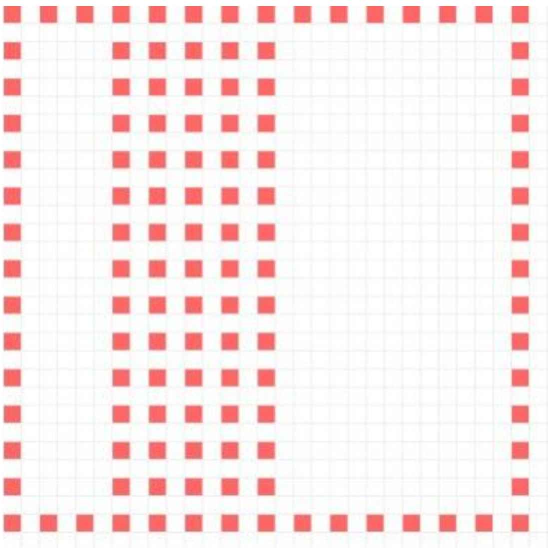


Layer 2

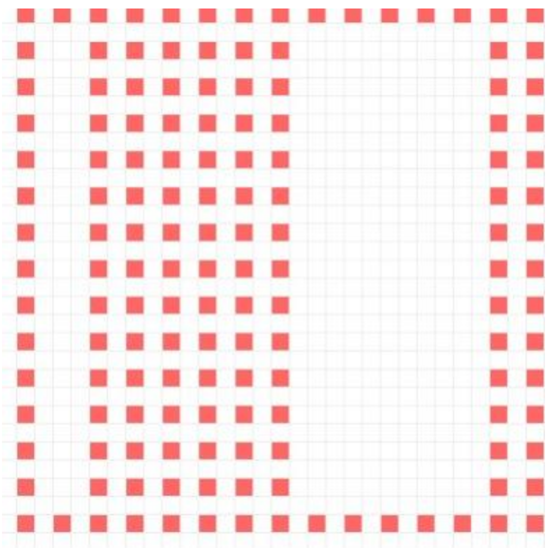


Layer 3

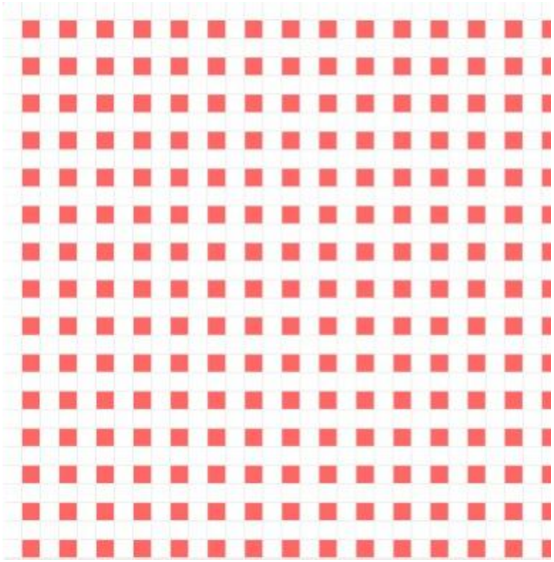
Time = 00:00:00:200



Layer 1

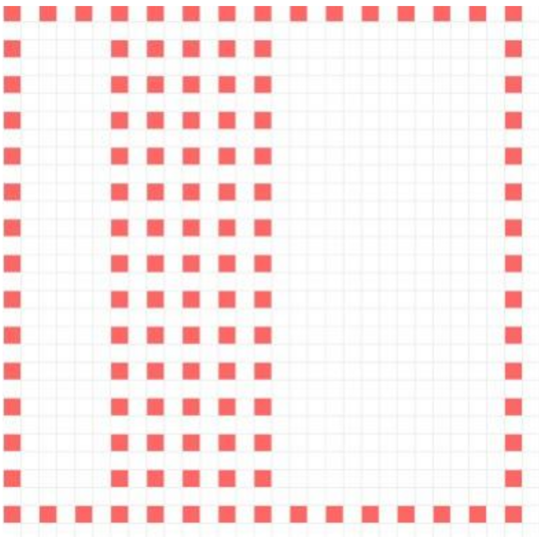


Layer 2

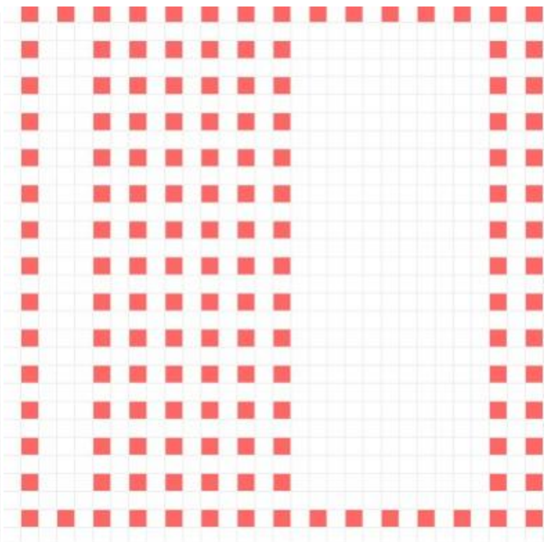


Layer 3

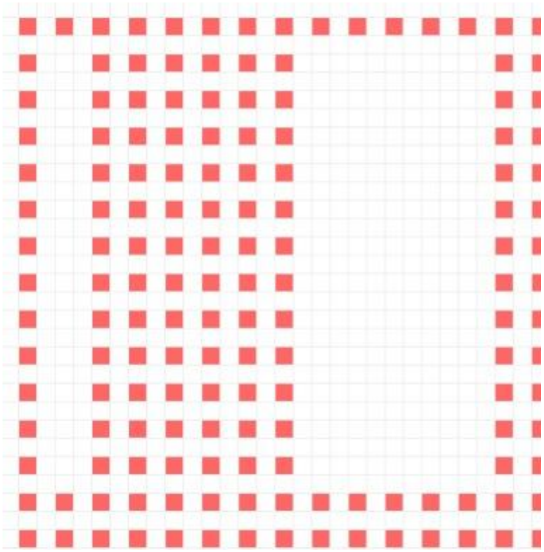
Time = 00:00:00:300



Layer 1

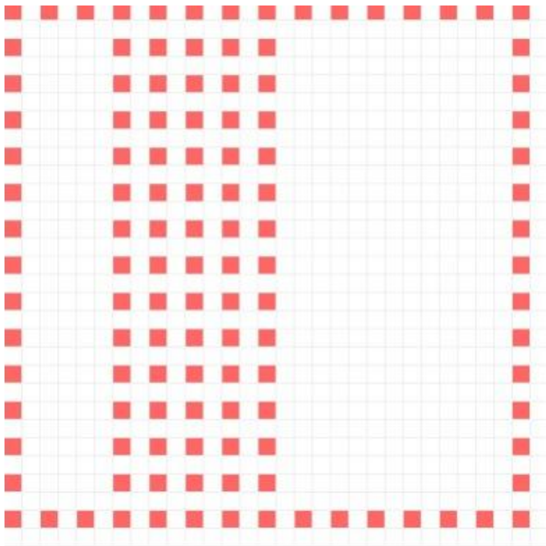


Layer 2

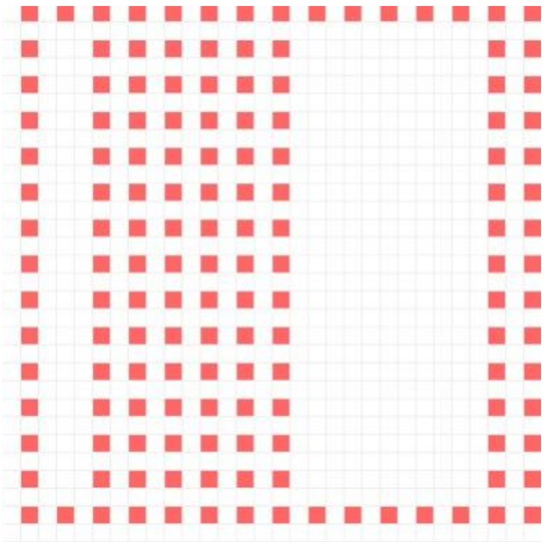


Layer 3

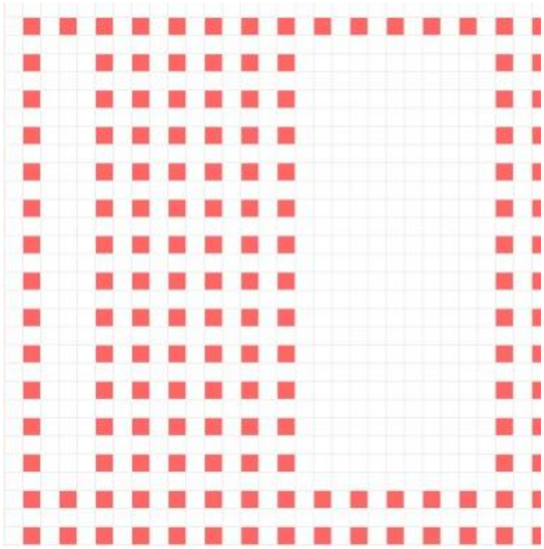
Time = 00:00:00:400



Layer 1



Layer 2



Layer 3

4. Conclusion

In our simulation, we regard Si etching as a Cellular Automata, which is discrete in time, space and state. Applying CD++ to simulate the Si wet etching can get a direct view of complex process quickly. Based on the result analysis, the virtual Si etching goes following the rules we defined and the final finish figure is as illustrated in theory analysis. But there are still some shortages: 1. Although we increase the model size, but the atom etching is in nanometer in practice, which is quite a large number and cannot be reflected fully in simulation; 2. We only simulate the V slot, anisotropy allows all kinds of pattern. So, we will continue to research the Cell_DEVS in etching with CD++ based on the current initial success.