Outline of Final Project

# Visualization Simulation of Nucleation on a Substrate

## Objective

The objective of the project is to construct a simulation of the nucleation process with an emphasis on a visualization of the process.

## Method

The simulation will be constructed using a javascript library called Paper.js which is a browser based technology capable of 2 dimensional graphics and mathematics processing. This, combined with standard HTML technology will allow the user to specify the parameters of the simulation, execute the simulation, visualize the nucleation process on a segment of the substrate as it occurs, and calculate the time it takes to cover the surface.

## Inputs

The inputs to the simulation should reflect the variables under the control of the technician growing the film. They include

* Temperature
* Pressure
* Deposit Rate

These are suggested parameters. Further analysis will be conducted to determine if they are appropriate and/or exhaustive. Alternatively, common elements can be displayed and chosen by the user, and the appropriate Deposit Rate calculated. This might limit or complicate the capabilities of the simulation.

## Simulation

Using the inputs, “dots” with a radius of 2 pixels will be deposited on the screen to simulation according to the deposit rate. They will move around in a random pattern at a speed according to the temperature. When 2 “dots” collide they will combine to form a larger dot. When a critical number of “dots” are combined, they will stay on the surface. Otherwise, after a calculated amount of time the dots will disappear, leaving the combined “dot”. The simulation will end when the dots are combined to fill up the entire surface.

## Results

The time it takes the simulation area to be completely covered by the dots will be reported as the results of the simulation. The user can then alter the parameters and re-run the simulation.

## Limitations

The 2D javascript framework, Paper.js, is a simple and powerful API for visualization of physical processes. However, it has some limitations, which will be common to all browser libraries.

* Spatial Resolution—the smallest achievable resolution is 1 pixel. A computer screen has the capability to display fixed amount of pixels, so the maximum amount of area is fixed and very small for a simulation of this type.
* Temporal Resolution—the framework will allow dynamics of its objects at a rate of approximately 60 times per second, but that is not a guaranteed rate. Therefore, at best, the smallest increment of time that can be used is 1/60th of a second.

## Calculations

The functions and factors for this simulation are estimated, and derived from considering Cu as the film to deposit and Si as the substrate. No particular reason. I just needed order of magnitude number.

#### Terms

Use Cluster and Molecule. Molecule, even though we are actually dealing with Atoms in my head.

### Scaling

#### Distance

Since the pixel is the smallest unit, I chose that length to represent 1 Angstrom

This is convenient since a Cu atom is 140 pm = 1.4 Å and an Si atom is approx. 240 pm = 2.4 Å.

#### Time

The time scale is

Where s is a second and S is a simulated second. In other words, for every 1 second the simulation runs, we observe 10-5 seconds of the nucleation process.

#### Temperature

Minimum = 0. Maximum = 1687.15 K (the melting point of Si)

Pressure

Ranges from -9 to 0

### Surface Area Comparison for Simulation Termination

Ideally, we’d compare the total surface area of each of the atoms with the total surface area of the substrate. However, because we are working with pixels and not continuous lengths, the reported area of the dots was much higher that their actual area. Therefore, I had to multiply the area of the drawing area by pi squared. That seemed to do the trick.

I figured that out by trial and error.

### Radius Calculation

When to atoms or clusters collide, they form a new cluster. The radius of the new cluster is based on the radius of the colliding atoms or clusters. It follows this formula.

### Desorption Rate

The documentation defines this s

We’ve identified Si and Cu as our “typical” elements involved in this simulation, but we don’t want to nail down a specific lattice frequency. The energy barrier is also highly dependent on the specifics of the system. Therefore, for this purpose, we will use the a typical residence time of 10-6 s.

I have decide, rather arbitrarily, that we want each atom to stay in the simulation for a maximum of 10 seconds simulation time. Therefore, we want 10-6 real seconds s to be 10 simulation seconds S

This is how I came up with the time scale used for the simulation.

The simulation runs 4 times per real second, so each step lasts .25 real seconds and simulates what would happen in .25 of 10-5 seconds.

Therefore, well use 10 as our maximum time to live.

### Surface Diffusion

Don’t do this

Ideally, we’ll use this formula

We’ve been using Si as our prototypical substrate element. The Atomic weight of Si is 28 amu.

That gives us the velocity in meters per second of an individual atom assuming all of its energy was kinetic. Its actual energy will be between zero and that value.

In our scale,

The simulation will run 4 processes per real Second S. Therefore

So, the maximum velocity of an atom per cycle

This will never work for us. Let’s try something else.

Statistical diffusion distance.

Our fallback method, to make it easier, we could follow this formula.

The atoms should move along the surface based on the temperature. Higher energy, from a higher temperature, dictates the motion. We want 0 K to result in no movement, and the max temperature of 1687.15 K (the melting point of Si) to result in the maximum possible movement of 550 pixels.

Therefore, the maximum motion per degree Kelvin is 3.067575 or just 3

Therefore, it should be

No. Don’t do that. DO THIS

Most are just one step. Just vary it between 1 and 4, since you are doing 4 steps per second. Here is your justification

We’ll assume that this substrate is perfectly smooth (no holes or steps, etc.) So the diffusion across the surface is equally likely in all directions. To simulate this, each atom can move up to 1 to 4 pixels per step, depending on the temperature.

Our temperature varies from 0 K to 1687.15 K (the melting point of Si), so the maximum allowed movement follows

* 0 K – 400 K : 1 pixel max
* 401 K – 800 K : 2 pixels max
* 801 K – 1200 K : 3 pixels max
* 1201 K – 1687.15 K : 4 pixels max

### Deposition Rate

For deposition rate we’ll use

Recall that 1 pixel is 1 angstrom. A Si atom is about 2 angstroms large, and each dot on the screen is about 2 pixels apart.

Therefore

450 pixels = 450 Angstroms = 4.5 e-6

The molecular weight of Si is approx. 28 amu. So

Where pressure is in torr.

That is for a single second. There are 4 steps per iteration. Therefore

## Prototype Screenshot