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.

## Algorithms

### Surface Area comparison

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

### Surface Diffusion

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,

Wrong. Update this with the information below in desorption rate

So, the maximum velocity of an atom per cycle

That isn’t right. We need to scale it down.

Alternatively, 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

### Desorption Rate

The documentation defines this s

We don’t really know a lattice frequency, and the energy barrier is also highly dependent on the specifics of the system. However, we can use a typical residence time of 10-6 s.

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

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.

### 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

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

Where pressure is in torr

## Prototype Screenshot