Visualization of Nucleation

A simple simulation of the Nucleation process for the purpose of visualizing how it works

Mark Watson

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# https://github.com/marklwatson/nucleation

# Objective

The objective of this body of work is to produce a visually observable simulation of the nucleation process in film growth, demonstrating the effect of temperature and pressure on the process. The results produced by the simulation are meant to approximate the behavior of the process, but are not intended to yield experimentally verifiable results. The goal is to produce a reasonably accurate visual representation of the nucleation process.

# Technology

The simulation is programmed using a 2D javascript graphics library called Paper.js which is a browser based technology capable of 2 dimensional graphics and mathematics processing.

<http://paperjs.org/>

The simulation is executed with a standard modern browser using HTML. The HTML code provides a facility for the user to specify the simulation parameters used for execution.

# Inputs

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

* Temperature (0 K to 1687.15 K)
* Pressure (10-9 Torr to 1 Torr)
* Critical Size (1 to 10)

Temperature and pressure are directly controlled by the technician. The critical size is controlled by the technician’s choice of material for the film. This simulation does not specify which materials are to be used for the film or for the substrate, so the critical size must instead be specified directly.

# Metrics

Scaling is required to execute the simulation in the javascript environment. The scaling factors are derived considering Cu as the film to deposit and Si as the substrate. This is not to simulate Cu film growth on Si specifically. It is only to provide orders of magnitude of estimated values.

The simulation is scaled spatially as follows

This is a decent approximation as a Cu atom is 140 pm = 1.4 Å and an Si atom is approx. 240 pm = 2.4 Å.

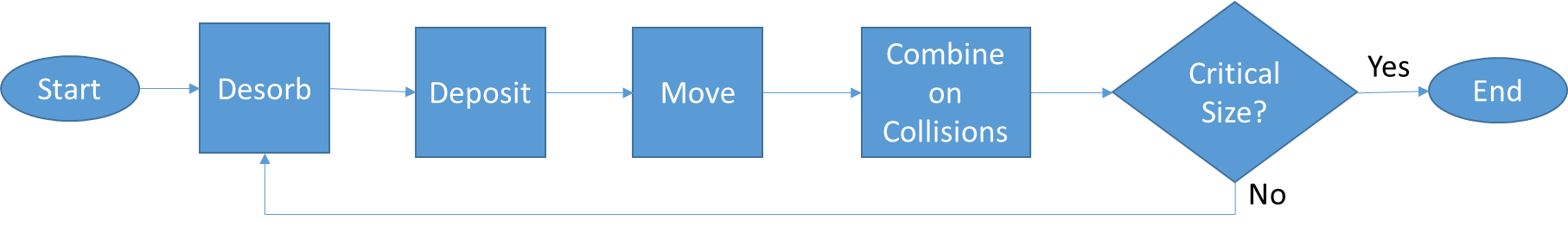
The simulation is scaled temporally as follows

where S is a second of simulation run time, and s is a second in the simulated nucleation process. I.E. 1 second of the simulation represents 10-5 seconds of film growth.

# Process

The simulation deposits molecules (atoms) onto the substrate at the calculated deposition rate. The atoms then diffuse across the surface randomly, but within a calculated maximum range. The atoms will either diffuse (leave the simulation) or they will collide with other molecules on the substrate to form a cluster. The atoms within the cluster can still diffuse until the cluster reaches the critical size. Once the cluster grows to that critical size its molecules will not diffuse for the remainder of the simulation. The clusters on the substrate continue to diffuse across the surface growing as they collide with molecules or with other clusters. Once one of the clusters reaches the termination size, the simulation is terminated.

The simulation is executed in a series of single process flows, or steps, iterating 4 times per second. The process flow is as follows.



* Desorb—any molecules on the substrate that are not a part of a cluster of critical size and have passed their residence time are removed from the substrate.
* Deposit—new molecules are deposited on the substrate at the calculated deposition rate.
* Move—molecules move in random directions at a random rate based loosely on temperature
* Combine on Collisions—when two molecules or clusters collide they combine to form a larger cluster
* Critical Size Determination—has any cluster on the substrate reached the critical size?

# Calculations

The factors used in the simulation are either statically specified or calculated based on the input parameters. The calculations determine the radius of a cluster, deposition rate, desorption rate, surface diffusion, and the termination condition.

## Radius of a Cluster

When two 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.

## Deposition Rate

The deposition is derived from the formula for the flux

Multiplying the area we can determine the deposition rate

The simulation is executed on an area of 450 pixels by 450 pixels. Recall that 1 pixel is 1 angstrom, so 450 pixels = 450 Angstroms = 4.5 e-6 . Additionally, the molecular weight of Si is approx. 28 amu. Therefore

Where pressure is in Torr and the temperature is in K.

That is for a single second. There are 4 iterations per second, therefore

## Desorption Rate

The book describes the desorption using the expression

The simulation does not specify a particular material for the substrate, so we don’t know the specific lattice frequency. The energy barrier is also highly dependent on the materials of the system. However, the book does specify a typical residence time of 10-6 s. That time will be used for the desorption rate.

It has been determined, rather arbitrarily, that each atom should stay in the simulation for a maximum of 10 seconds simulation time. Therefore 10-6 seconds of residence time will be 10 seconds S of simulation time. As already noted

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.

## Surface Diffusion

The simulation assumes that the 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 will move up to 1 to 4 pixels per step, depending on the temperature.

The variation of the motion based on temperature is as 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

## Termination Condition

The simulation will terminate when a single cluster covers 75% of the surface area of the substrate

# Results

The time it takes the simulation area to be completely covered by a single cluster is 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.
* Coordinate System—the rows and columns nature of the pixels makes use of radial calculations more difficult.

# Improvements

* Materials for the substrate and the film material could be specified.
* Using this, precise calculations could be made for deposition rate, desorption rate, surface diffusion, and critical cluster size
* Common material configurations can be provided and chosen by the user to provide the values for the above calculations.
* Different lattice configurations of the substrate can be taken into account.
* Different colors for the substrate and the film material could be picked

# Screen Shot

