Heteroepitaxial Growth Using Off-Lattice KMC

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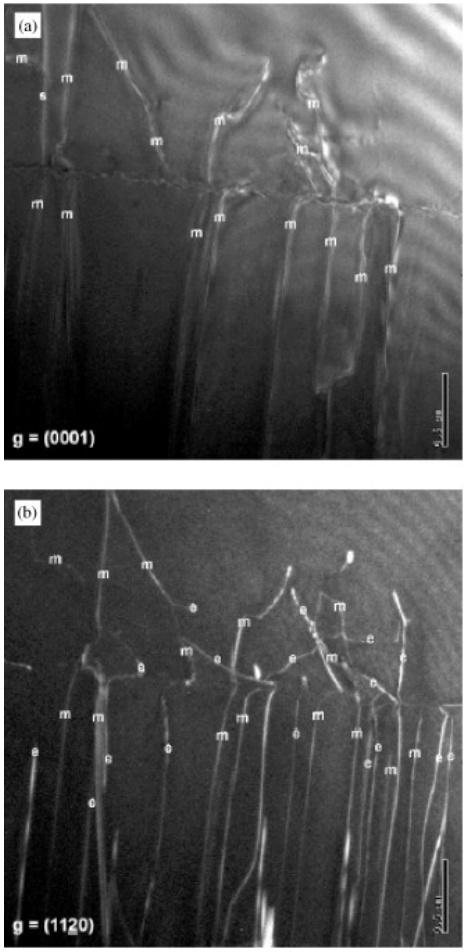
Why Heteroepitaxy?

- Difficult to Model
  - Multiple Species
  - Dislocations and point defects important
  - Species Flux important
- The Silicon Age is Ending
  - New materials and growth required
- Useful in design of Devices
  - $$$

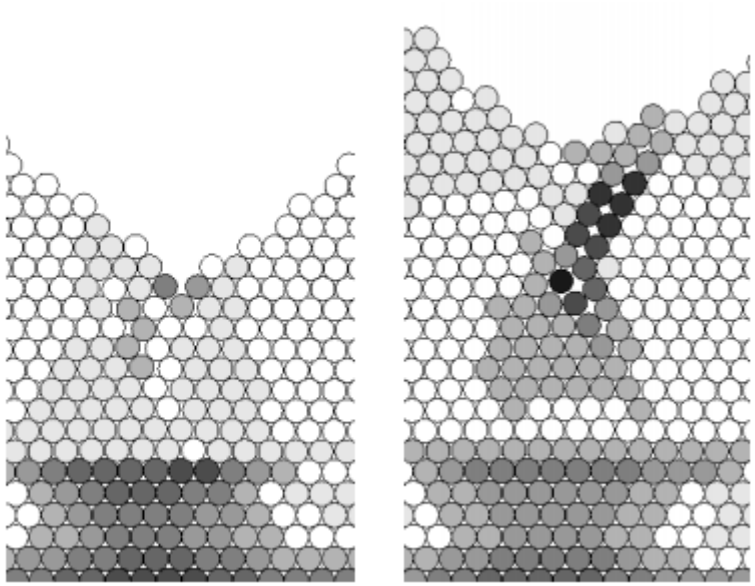
Motivation for Off-Lattice KMC Heteroepitaxy

- Lattice fixed atoms have restricted motion
- Inability to classify defects such as dislocations
- Defects play a tremendous role in semiconductor device performance
- “Strain” between multispecies interfaces cannot be accurately classified with on-lattice KMC



http://www.sciencedirect.com/science/article/pii/S0022024804003112

Previous Work



$\epsilon = -.5\%$

- Biehl (2004)
  - Heteroepitaxy
    - Particles differ in size
    - Leonard-Jones Potential
  - KMC
    - Time scale too long for MD
  - Off Lattice
    - Strain Relaxation
    - Dislocation formation
    - Diffusion

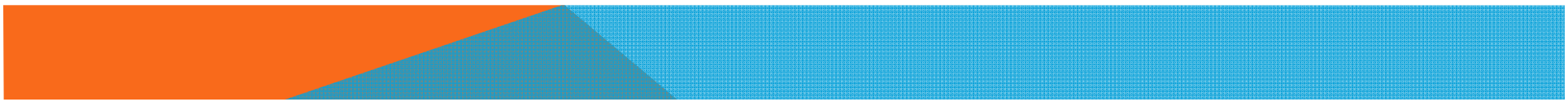
Off-Lattice KMC algorithm

Initialization:

- Initialize substrate
- "Bin" atoms
- Initialize rate catalog
  - Find 'free' atoms
  - Find Potential Energy Surface (PES)
  - Calculate rates to local minima in PES

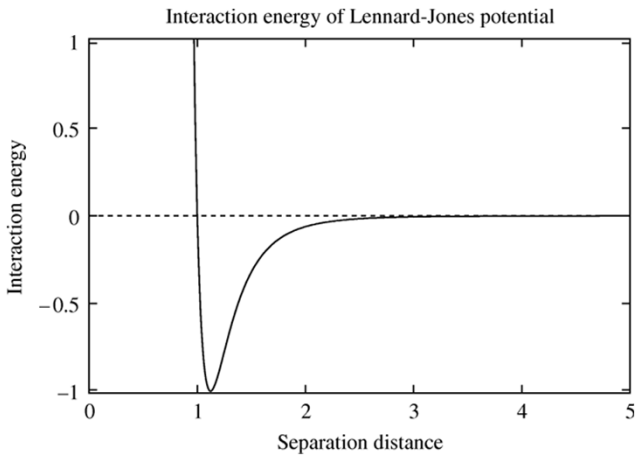
Main loop:

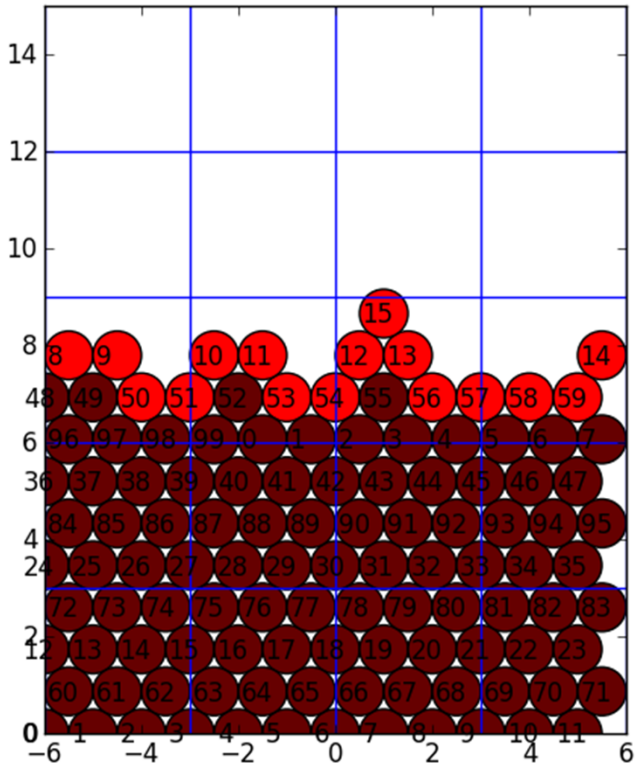
- Choose a move from the rate catalog
- Deposit an atom/make a diffusion move
- Perform local relaxation
- Update "binning" (local update)
- Update rate catalog (local update)
- …repeat over and over again…



Atom “Binning”

- L-J interaction falls off rapidly and becomes negligible at distances > 3σ
- Consider only particles in a neighborhood region when calculating forces, energies, and for determining which rates need to be recalculated after a move has been made
- Fast identification of surface atoms





http://www.emeraldinsight.com/content_images/fig/3980020402014.png

KMC: N-Fold Rate Catalog

- KMC rate catalog made from surface atom PES scan and deposition rate

$$R_{Deposition} = \left(\frac{L_{substrate}}{a_s}\right) * \frac{Monolayer}{s}$$

$$R_{Diffusion} = v_0 * \exp\left(-\frac{\Delta E}{kt}\right)$$

$$where\ v_0 = 10^{12}/s$$

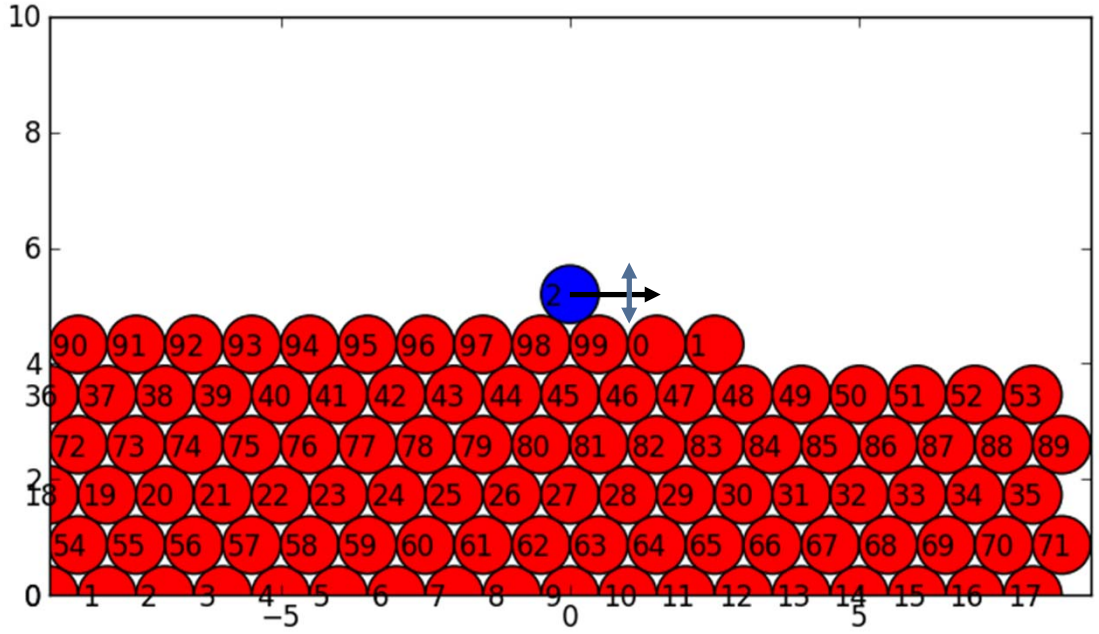
- Catalog is scaled according to total rate
- Random number 0-1 is chosen
- Bisection search algorithm chooses event

Event	Barrier Height ΔE	Final Position
Atom 1: Move Left	ΔE1	X1
Atom 1: Move Right	ΔE2	X2
Atom 2: Move: Left	ΔE3	X3
Atom 2: Move: Right	ΔE4	X4
.	.	
.	.	
.	.	
Deposition	-----	Xn

0

1

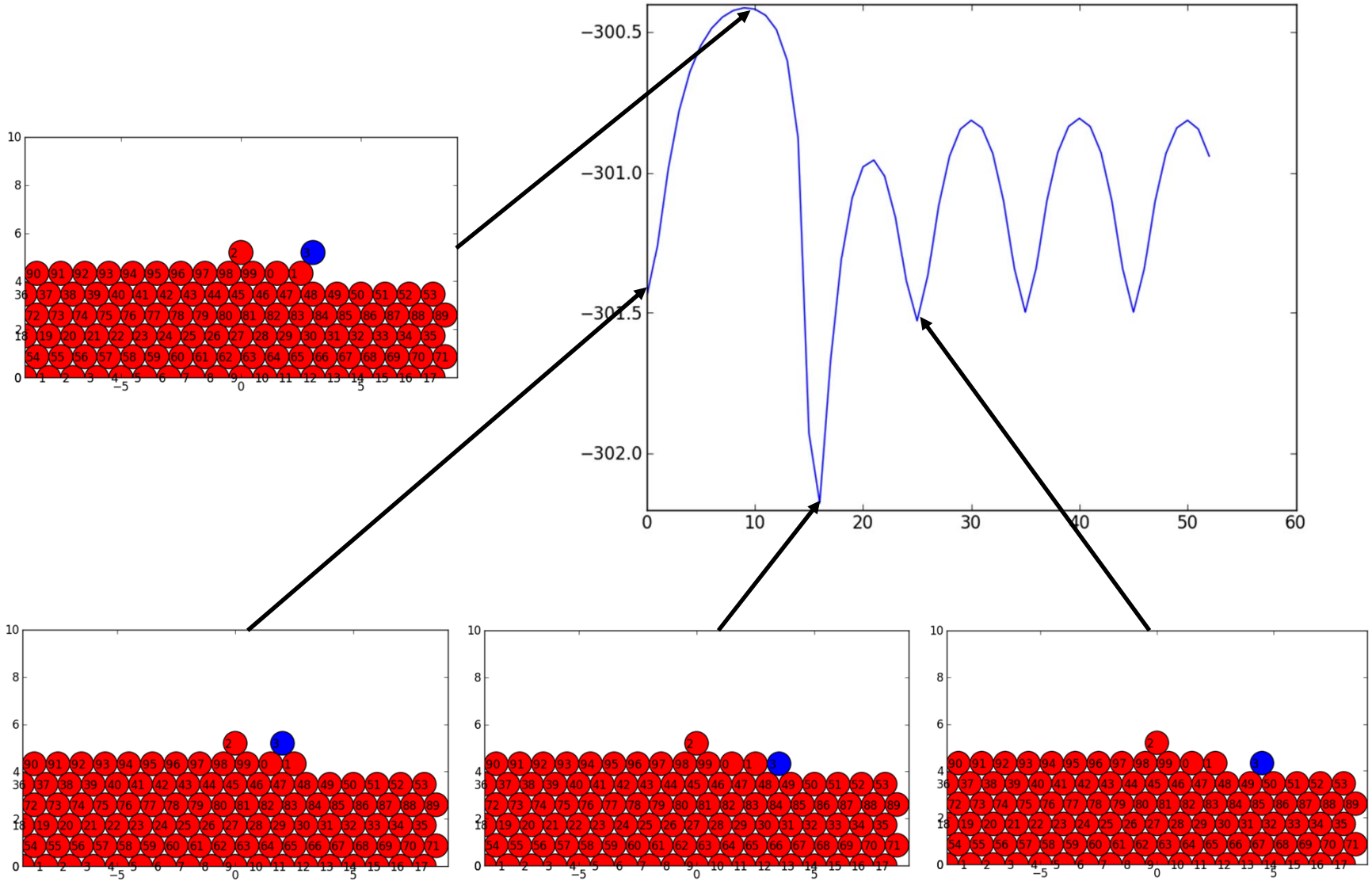
Generation of PES – Making a virtual move



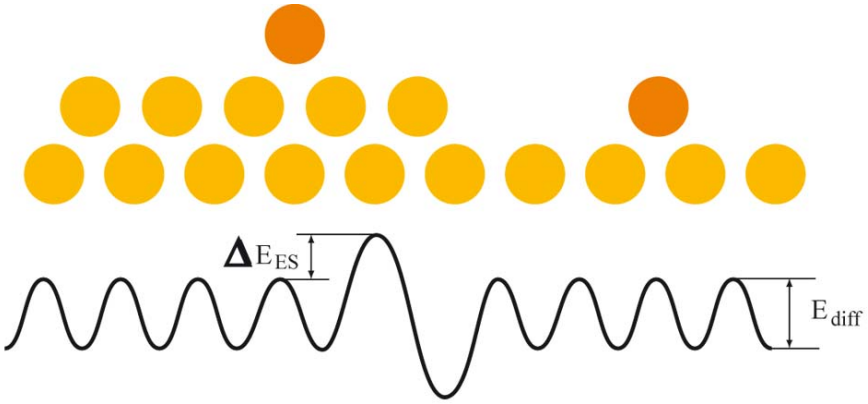
Move atom slightly along the x-direction

Minimize energy with respect to the atom's y-position
(using "frozen crystal approximation")

Generation of PES



Physics behind it…Ehrlich–Schwoebel barrier

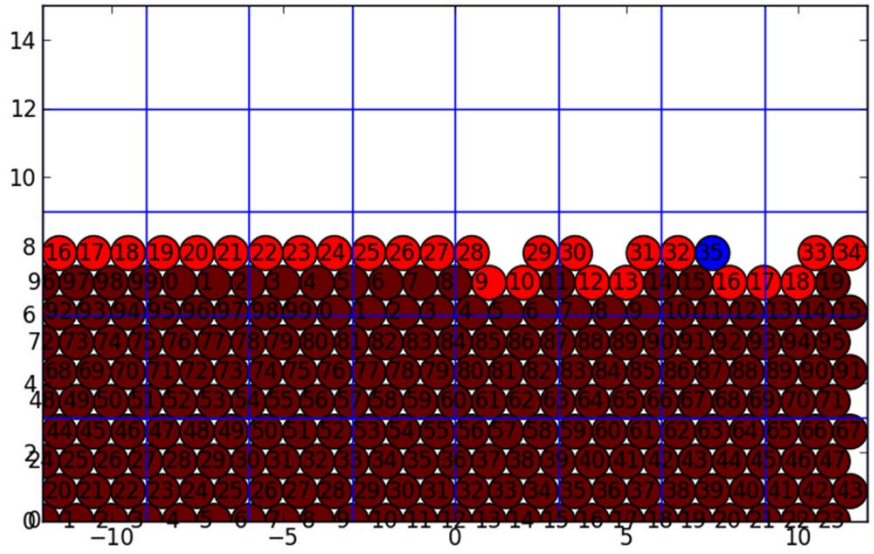


http://eng.thesaurus.rusnano.com/upload/iblock/ebd/ehrlich-schwoebel-barrier.jpg

- Atom approaching the step on the lower side has a lowered energy barrier to attach to the step → site at the step has a larger number of nearest neighbors
- Atom approaching the step on the top side faces an additional energy barrier ΔE_{ES}, known as Ehrlich–Schwoebel barrier → has to pass through a state with a low number of nearest neighbors in order to cross the step edge

Deposition Event

- Surface atoms are identified from surface bins
- Atom is placed on top of and either to the left or right of a randomly chosen surface atom
- Atoms are relaxed to local minimum with molecular statics



Molecular statics relaxation

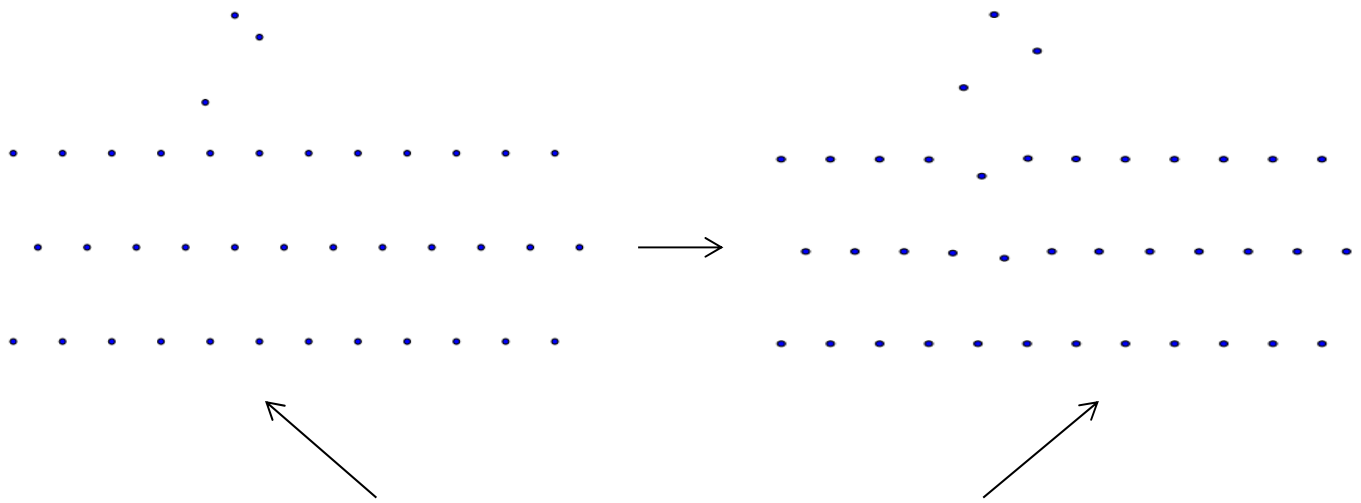
Conjugate Gradient Minimization Algorithm

- $\Delta x_0 = -\nabla_x f(x_0)$
- Perform Initial Line Search: Determine α_0 for x and y direction of each atom such that $f(x_0 + \alpha \Delta x_0)$ is minimized
- Update Positions: $x_1 = x_0 + \alpha_0 \Delta x_0$
- Initialize Conjugate Direction: $s_0 = \Delta x_0$
  1. Determine the Steepest Direction: $\Delta x_n = -\nabla_x f(x_n)$
  2. Determine Conjugate Direction Step Size β_n According to Polak-Ribiere Formalism: $\beta_n = \frac{\Delta x_n^T (\Delta x_n - \Delta x_{n-1})}{\Delta x_{n-1}^T \Delta x_{n-1}}$
  3. Update the Conjugate Direction: $s_n = \Delta x_n + {}_n s_{n-1}$
  4. Perform Line Search: Determine α_n for x and y direction of each atom such that $f(x_n + \alpha \Delta s_n)$ is minimized
  5. Update Positions: $x_{n+1} = x_n + \alpha_n s_n$
  6. Repeat 1-5 Until Forces on All Atoms are Sufficiently Small

Molecular statics relaxation of simple system

Initial Configuration

Relaxed Configuration



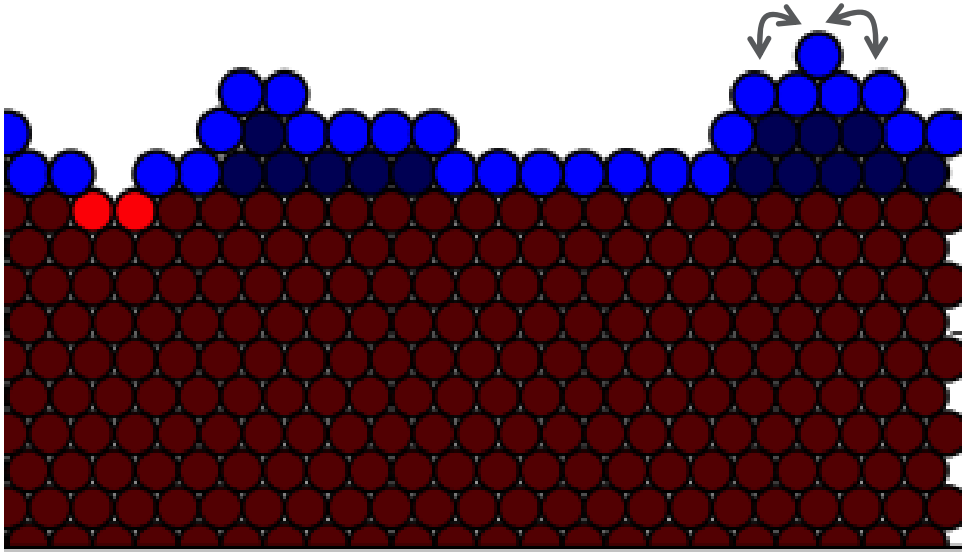
Fixed Positions on Bottom Row

Adaptive KMC

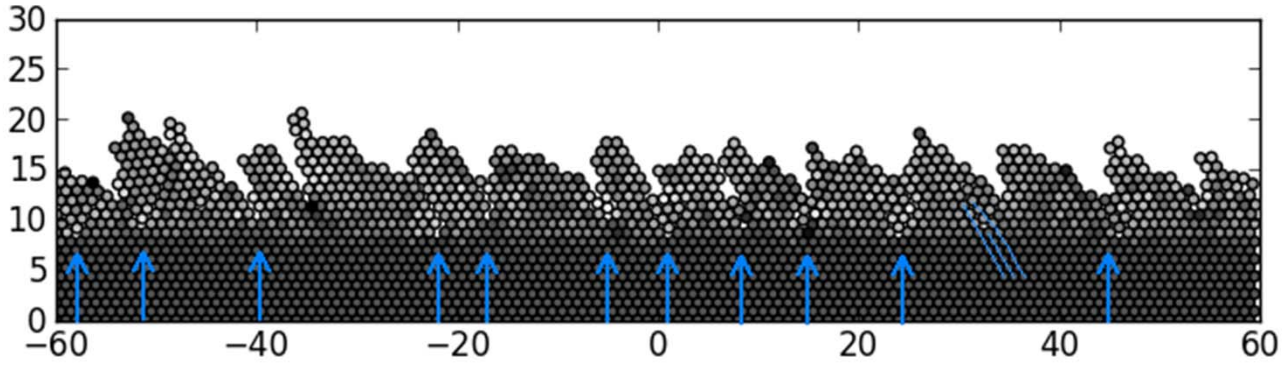
- Oscillation between states
  - See it in Action!
  - Rate $\propto \exp(-\Delta E)$
  - ΔE is small, rate blows up
  - Moves between these states dominate all others
  - No evolution in system

- Solution
  - Scale Rate by $\exp(-\kappa N)$
  - κ = Damping Constant
  - N = number of times move has occurred before

- Ideal Solution
  - Combine states into superstates
  - High programming cost

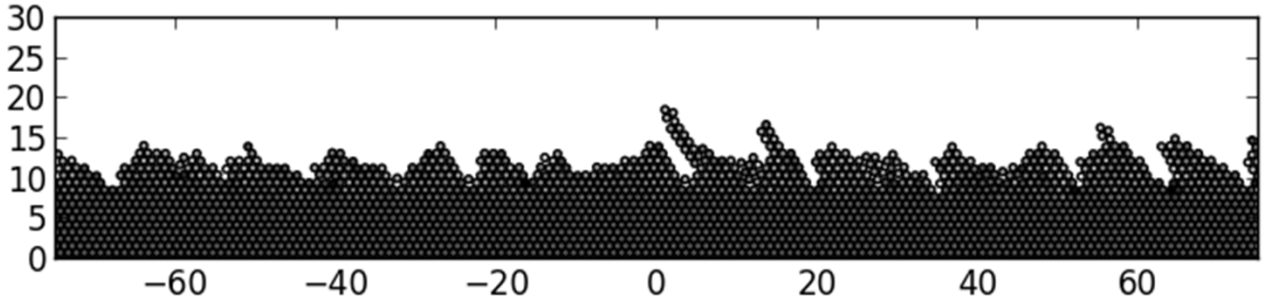


Results: Two Species System Video



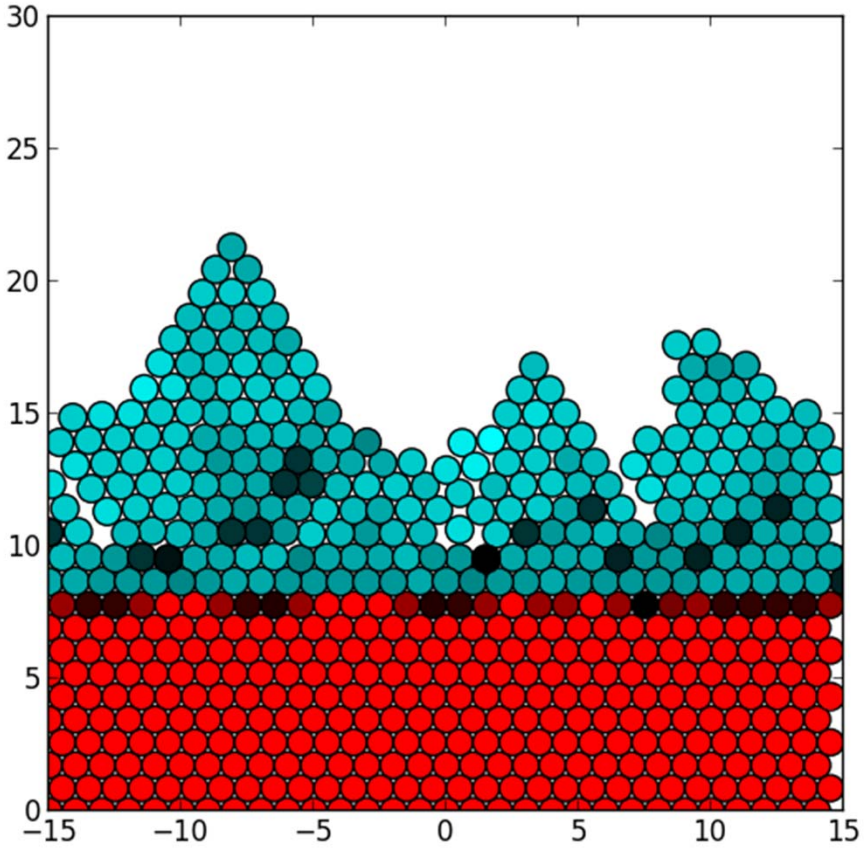
- Substrate Lattice Constant: 1.0
- Film Lattice Constant:1.05
- http://www.youtube.com/watch?v=i3dCXWubuFw

Results: Two Species System Video



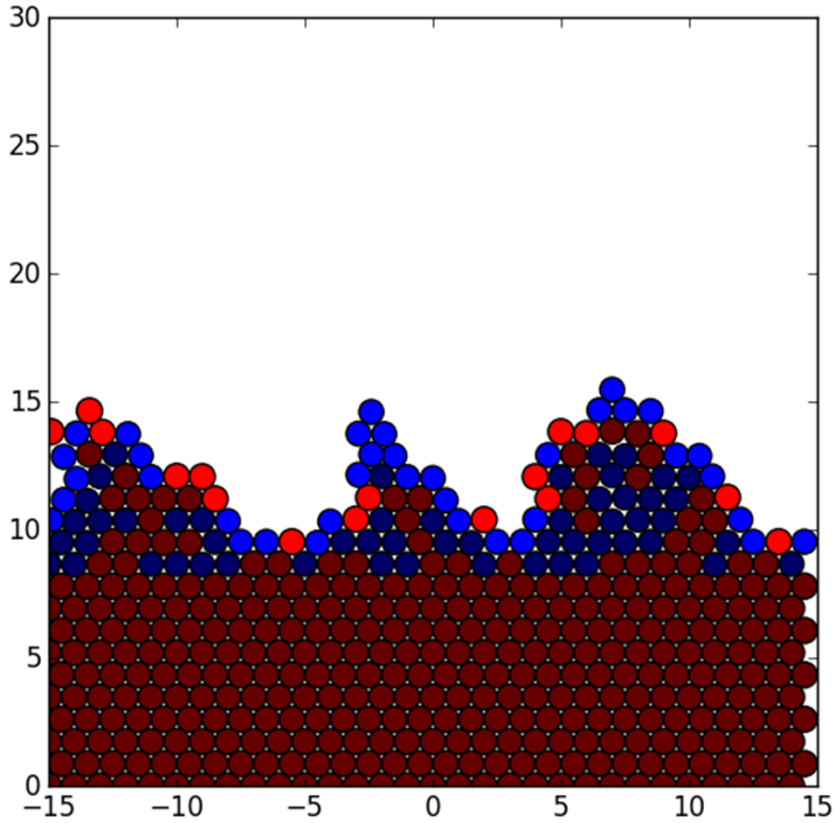
- Substrate Lattice Constant: 1.0
- Film Lattice Constant:0.95
- http://www.youtube.com/watch?v=Fec6yvWzam8

Classifying Strain/Defects:



- Color map based on average neighbor interatomic distance

Extending this model: Multi-Species Deposition



- Random probability of depositing both species

Future Work/Questions

- Model shows reasonable results: Dislocations can be classified
- Increase system size for 2D
- Extend to more complicated potentials
- Extend to three dimensions
- Questions???