Computer Tutorial: KMC Simulations of the Solid surfaces

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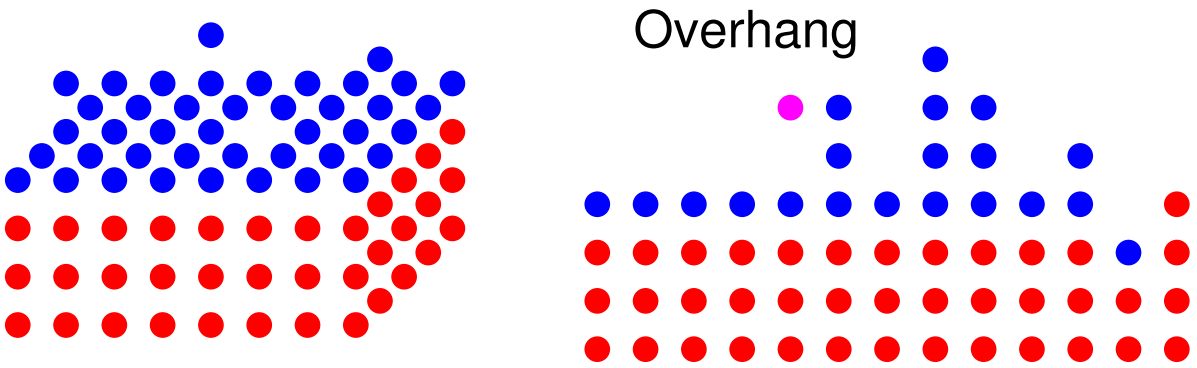
Outline

- Solid on Solid Model
- Monte Carlo simulations
- KMC simulations - Dynamics - Nonequilibrium Processes - Crystal growth
- Rejection free methods

Solid on Solid Model

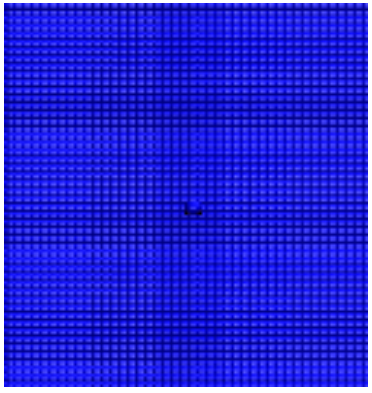


SOLID ON SOLID MODEL

- Used to model crystalline lattice systems
- Preferred direction of growth defines a surface
- This surface is modeled by a discrete variable $h(x, y)$ where x,y form a lattice
- No overhangs, so $h(x, y)$ is a good variable

Maps to a 2-D Potts model, Roughening Transition at a temperature T_R in the Kosterlitz-Thouless universality class of 2D phase transitions.
Chui and Weeks, *Phys. Rev. B.*, **14**, 4978 (1976)

Roughening Transition



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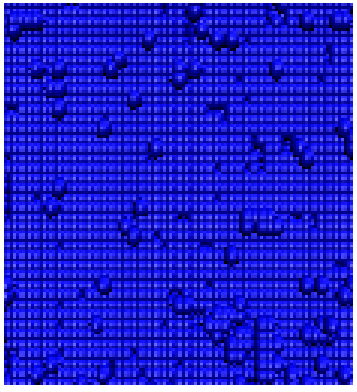

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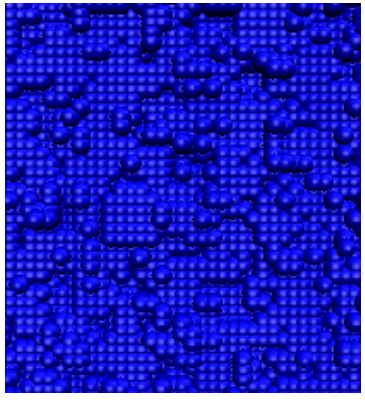

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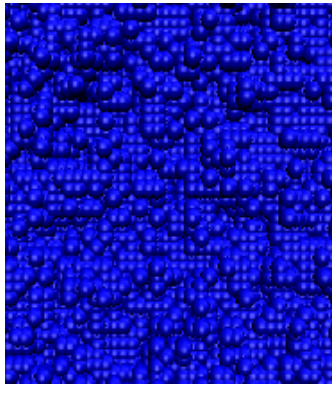

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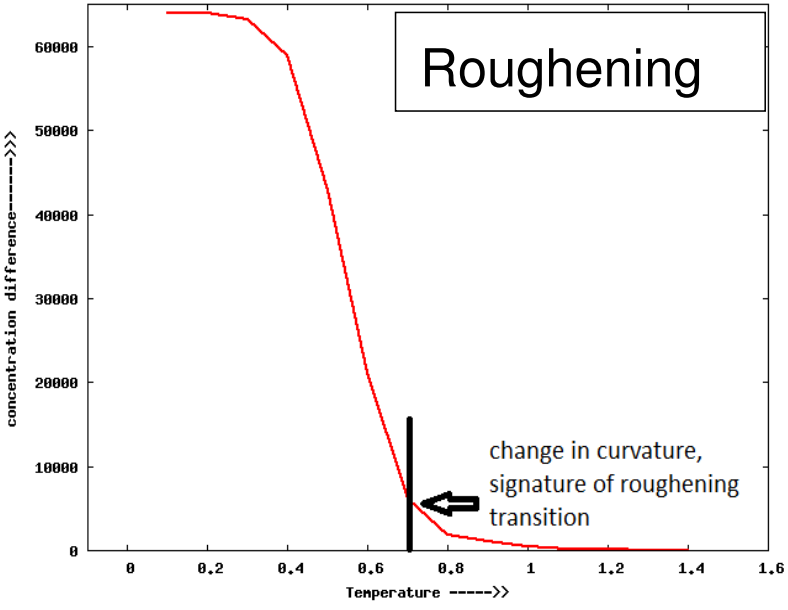
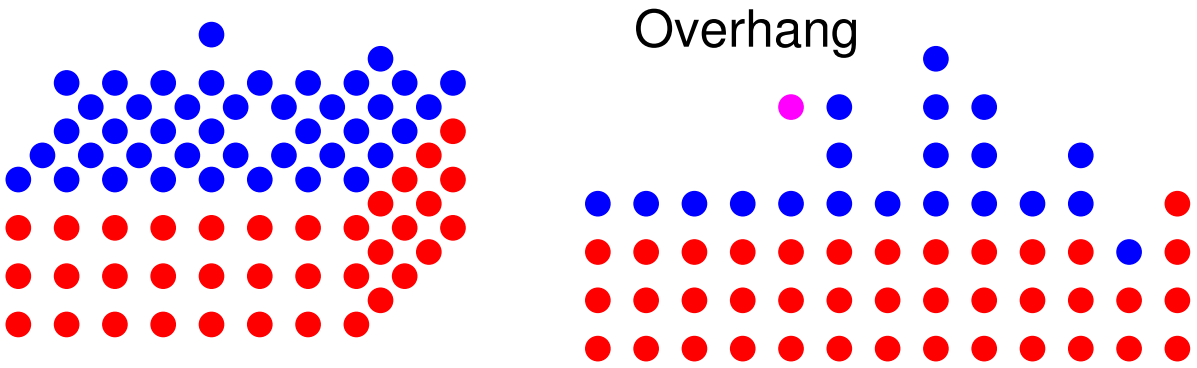


Monte Carlo simulations

- Fundamental process being modeled is surface diffusion of atoms
- Random motion of surface atoms
- Attempt to move atoms on the surface to their neighbouring sites
- Acceptance according to the Metropolis criteria
- Energy of a configuration is related to the number of bonds

Energy changes are purely local quantities involving atom under trial and its neighbors

KMC Simulations - Solid on Solid Model



SOLID ON SOLID MODEL

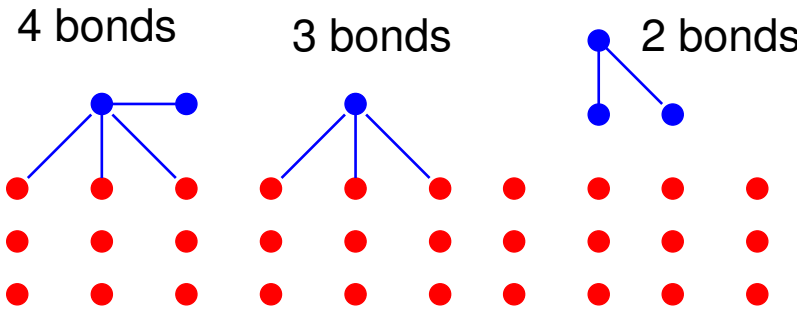
- No overhangs, atom must have another atom below it
- Select a surface atom and try to move it
- If accepted, move to a neighboring site
- Can have more elaborate methods -
  allow more moves, more complicated barrier relations

KMC simulations

- KMC simulations - Accept Moves with acceptance probability

$$p_{acc} = e^{-E_b/kT}$$

- Hopping barrier calculated by no of broken bonds - Example - Nearest and Neighbor interactions



Broken Bond Energetics

- Rejection-Free algorithm
  A.B.Bortz, M.H. Kalos and J.L. Lebowitz, J.Comp. Phys. (1975)

Rejection-Free KMC: Classes of moves

- A surface atom can have between 1 and 17 bonds so there can be 17 classes of molecules if all the bonds are identical
- Pre-processing: Assign classes to all surface atoms
- Count no of atoms in each class- Total Probability - $Q = \sum_i^{classes} N_i P_i$
- Generate a random number between 1 and Q. Based on the value of this random number, one particular class is selected; and then one atom in the class
- Class search can be efficiently done using a binary tree search algorithm
- Once atom is chosen, it can be moved to any neighboring site and time is updated according to the BKL procedure.

KMC simulations for a two component

- Two folders named kmc and bkl
- varaibles.h describe conditions under which these simulations are done
- Change to bkl directory. Compile: gcc -lm kmc.c -o kmc
- Run: ./kmc
- Analyze output:
  vmd initialstate.xyz
  vmd finalstate.xyz
- Repeat for directory bkl, now there is a time associated with each kmc step
  gnuplot Timefile.gnu