Lattice Kinetic Monte Carlo: Building a bridge between *ab-initio* calculations and process simulation

Polycrystalline Materials

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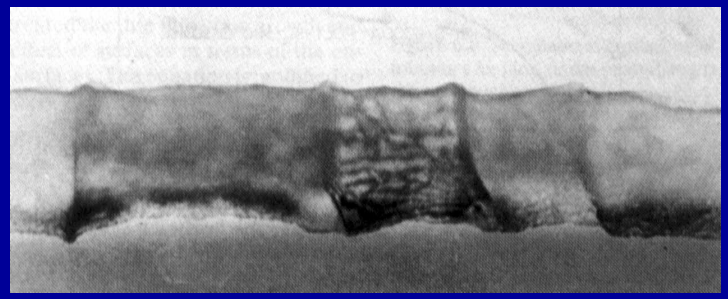
Why **Lattice** KMC?

Aluminum, Polysilicon, …: Polycrystalline structure

100 nm



0.5 µm

- Kang et al, J. Electron. Mater. , 1997
- Murarka, “Metallization”, 1993

- Surface texture
- Grain Boundary diffusion
- Electromigration

} depends on: deposition rate, temperature, substrate

Simulation approaches

- Continuum equations:

  SPEEDIE, SAMPLE, EVOLVE, DEPICT

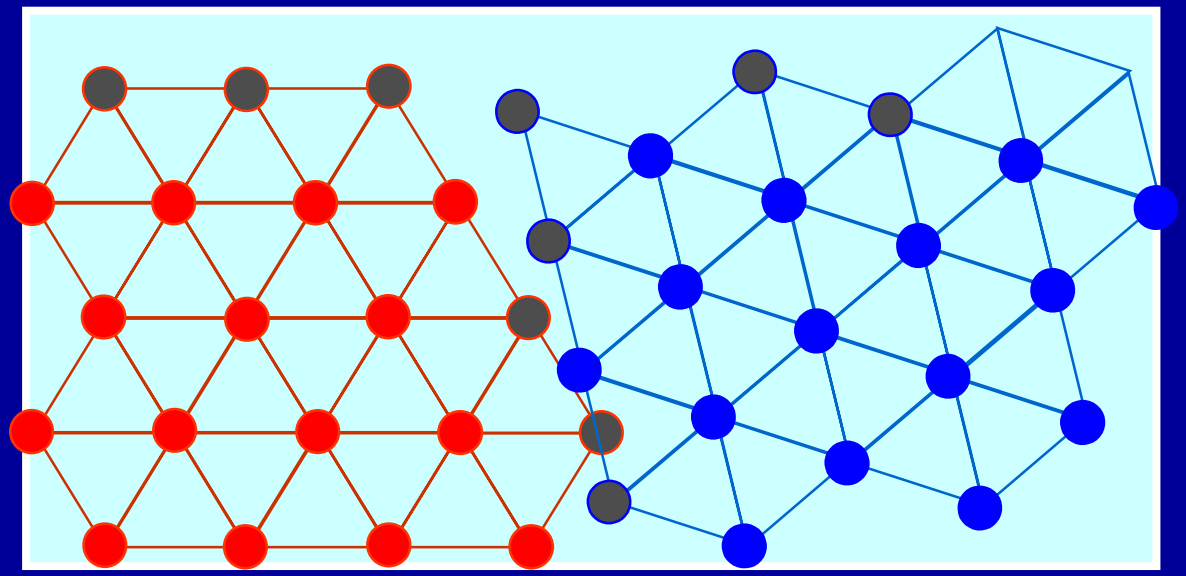
- 2-D ballistic simulator:

  SIMBAD, GROFILMS

- 3-D atomistic approach: ADEPT

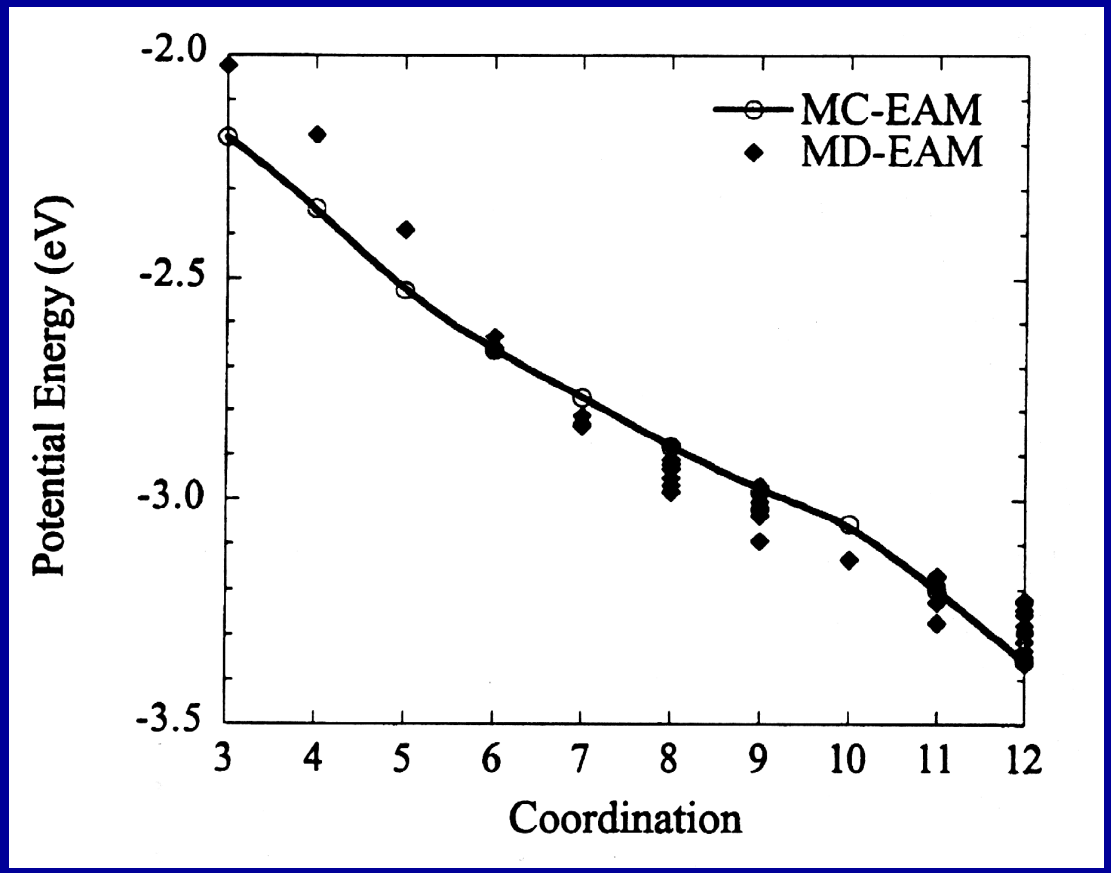
This Work: Polycrystalline 3-D atomistic approach

Simulation Box

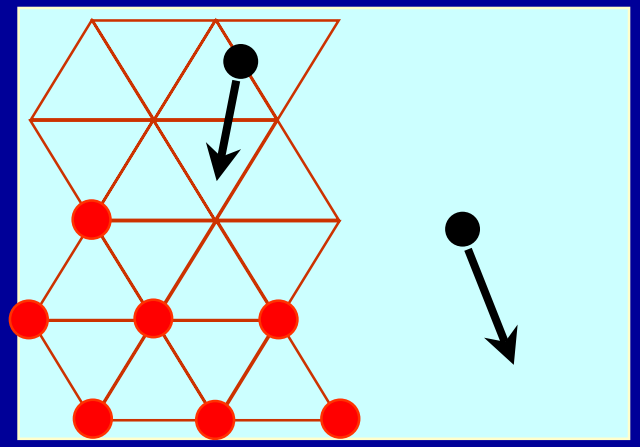


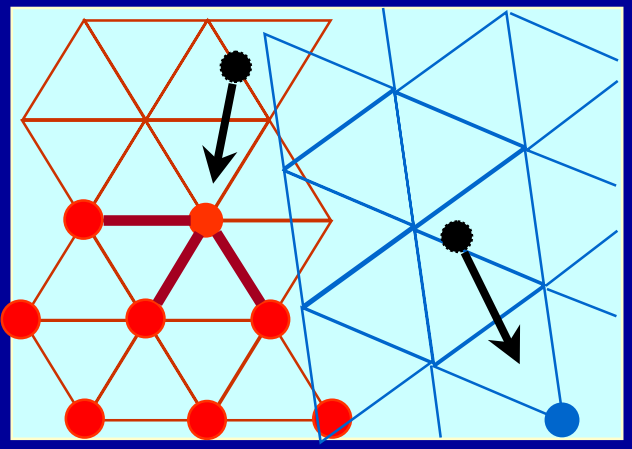
- Atoms are attached to the sites of a perfect fcc lattice.
- As a first approximation, the binding energy of each site depends on the number of occupied nearest neighbors

Energies from MD Embedded Atom Method using Gupta Potential



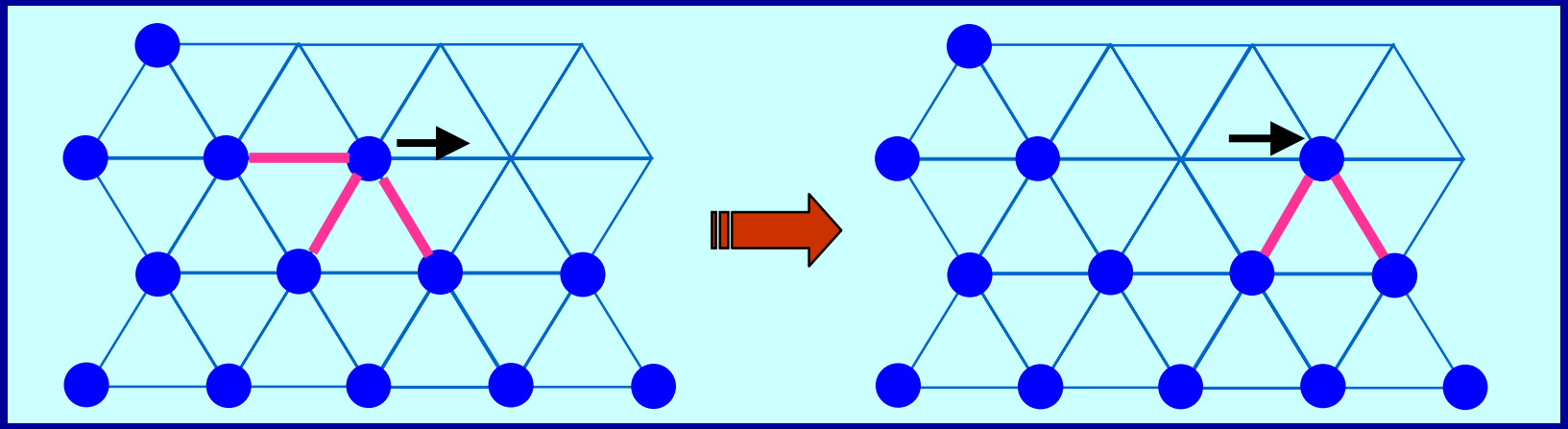
Deposition





- Initial position and velocity according to desired distribution
- Atom travels in a straight line until it either:
  - Finds some neighbors: gets attached to that grain
  - Finds no neighbors: starts a new grain (orientation).

Surface Diffusion



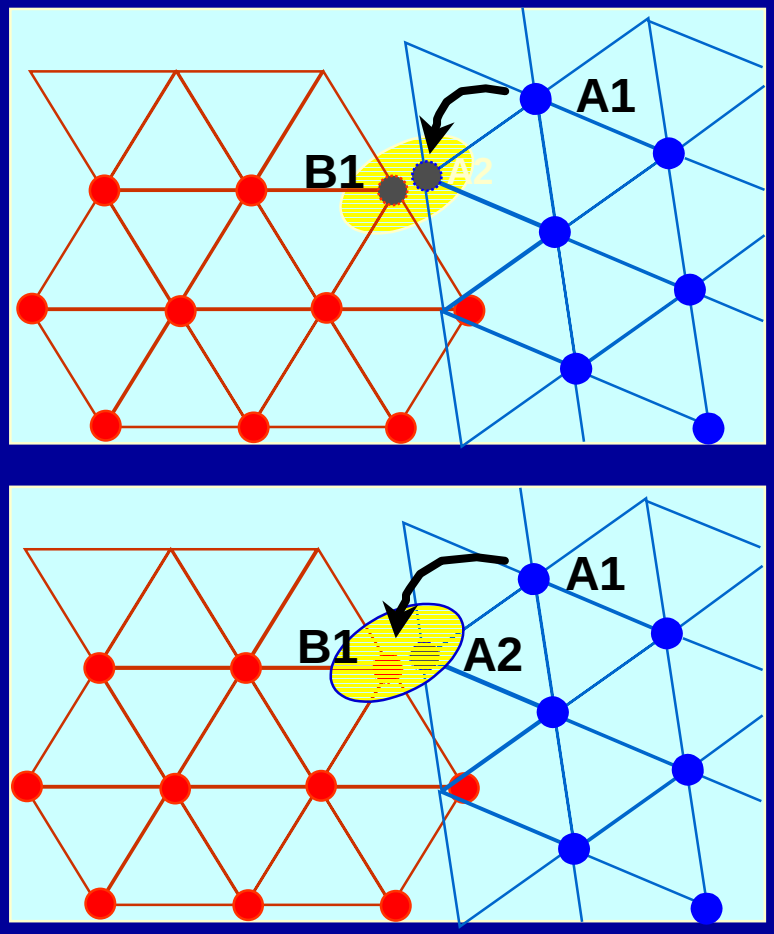
- Atoms not fully coordinated can jump to a neighboring empty site.
- The jump probability depends on the number of nearest neighbors and on the migration energy.

Grain Boundaries

If the destination site of a jump (A2) is at a grain boundary:

1. Check the energy of sites belonging to other orientations (B) around destination site.

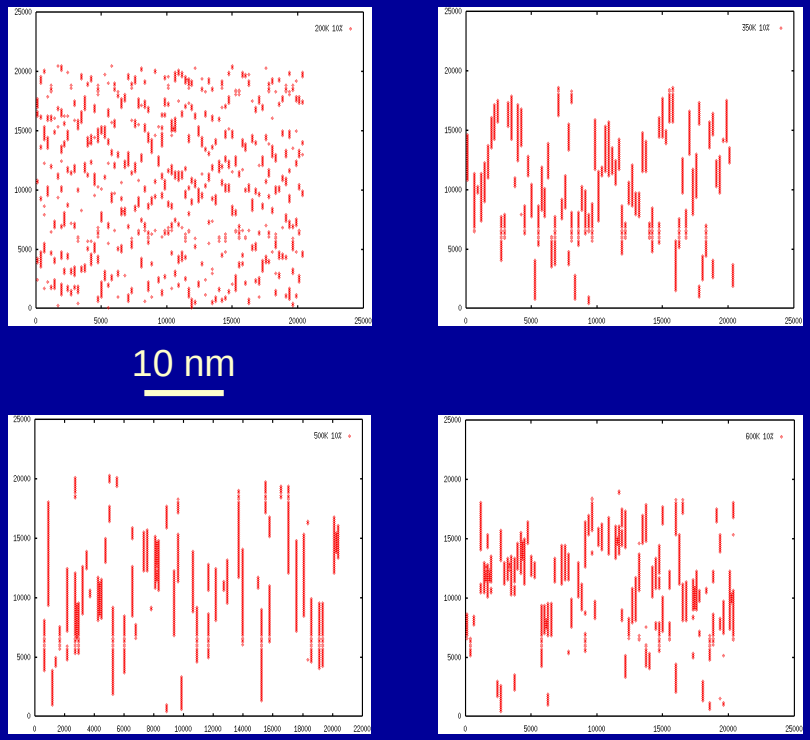
2. If energy (B1) < energy(A2) then the jump final site is B1.



Lattice KMC: Simulation Examples

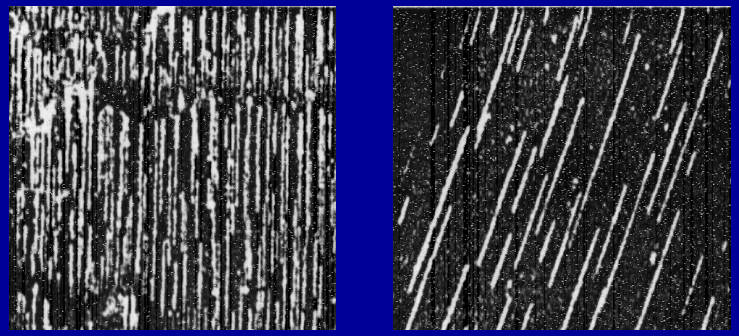
- Nucleation
  - Crystalline Substrates: Orientation
  - Amorphous Substrates: Wetting
- Annealing:
  - Texture evolution

Nucleation on Al (110)



10 nm

Simulation:
Al on Al (110) @ 200K, 350K, 500K, 600K
Coverage=0.1 ML

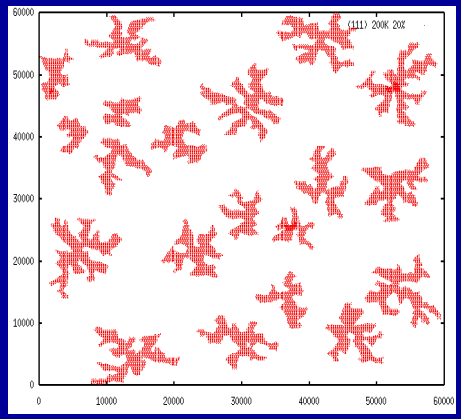


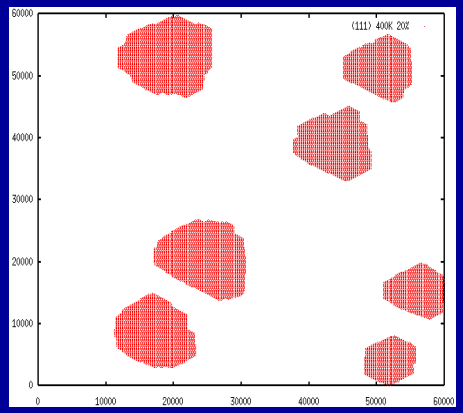
50 nm

STM images of Cu islands on Pd(100) at 265K and 300 K and coverage of 0.1 ML and 0.07 ML

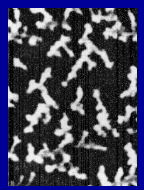
Nucleation on Al (111)

Simulation:
Al on Al (111)
@ 200K and 400K

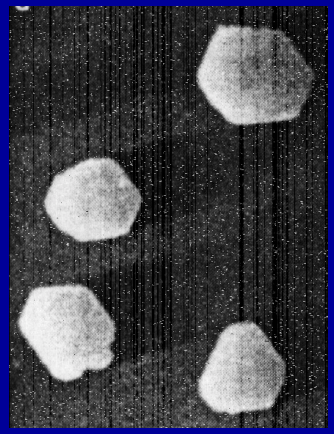




STM measurements:
Pt on Pt(111)
@ 200K and 455K



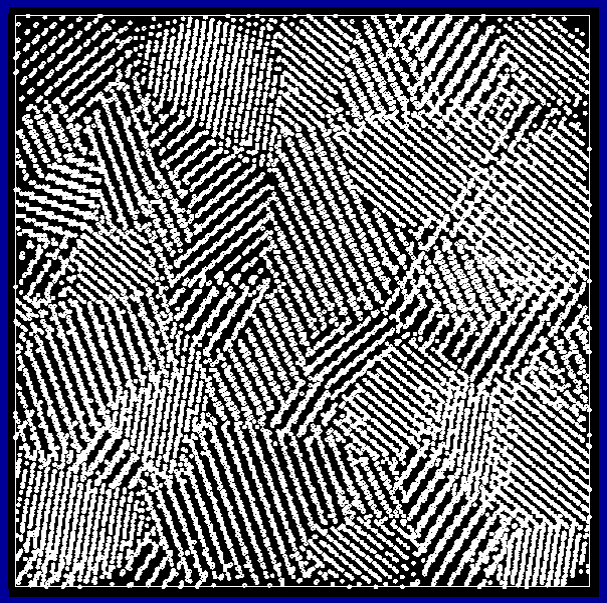
20 nm



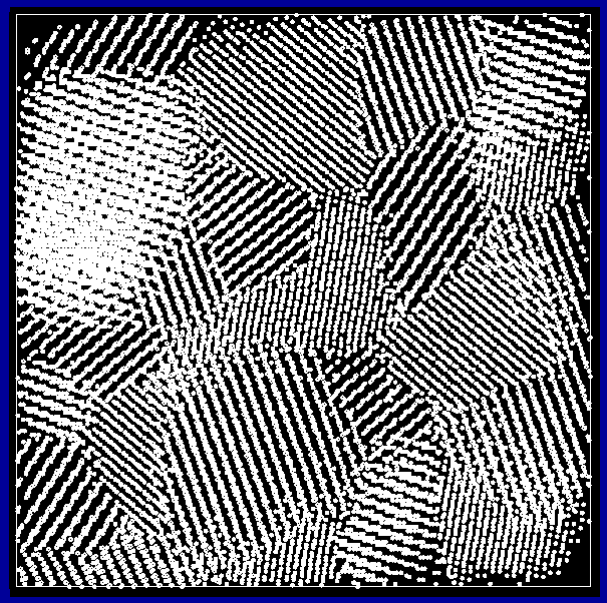
20 nm

Nucleation on Amorphous Substrates

Bonding to substrate: effect on the grain size

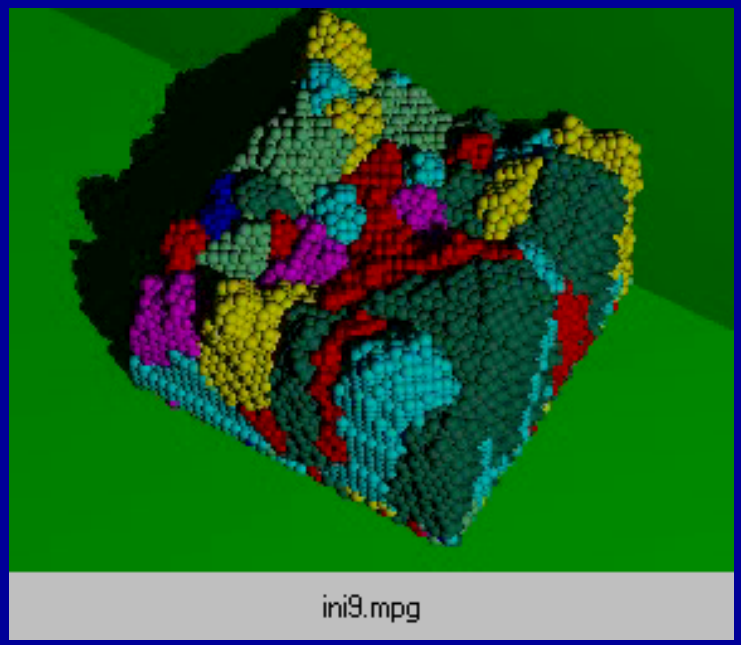


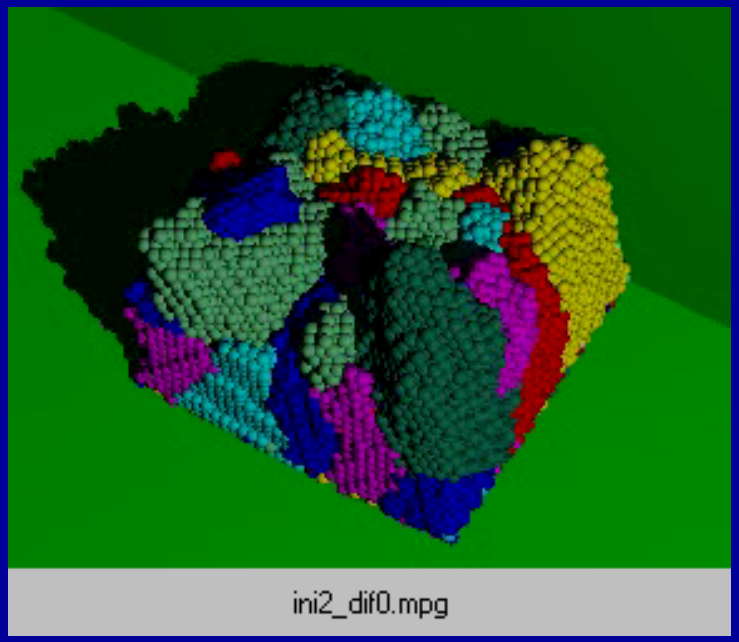
“Wetting” substrate
(Strong bonding)
=> smaller grains



“Non-wetting” substrate
(Weak bonding)

Nucleation on Amorphous Substrates





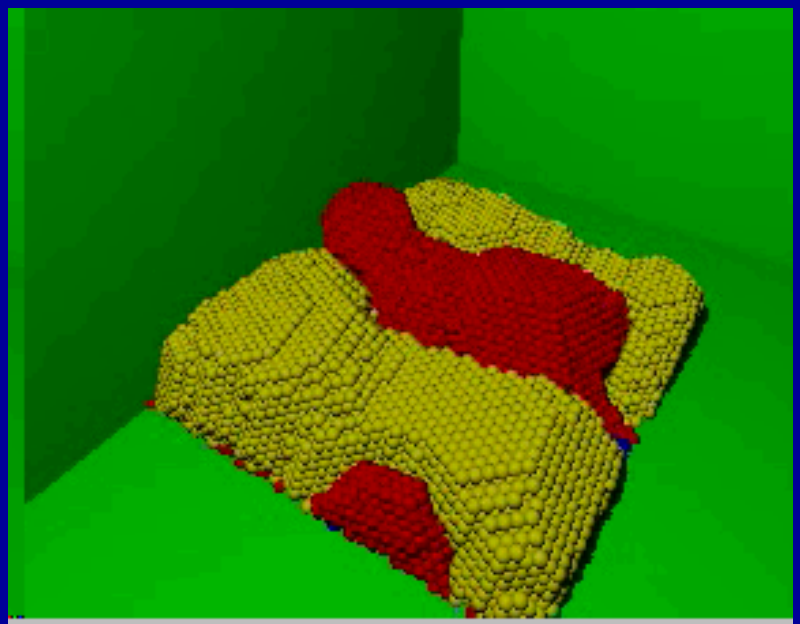
“Wetting substrate”
(Strong bonding)
=> smaller grains

“Non wetting substrate”
(Weak bonding)

Annealing: Texture Evolution

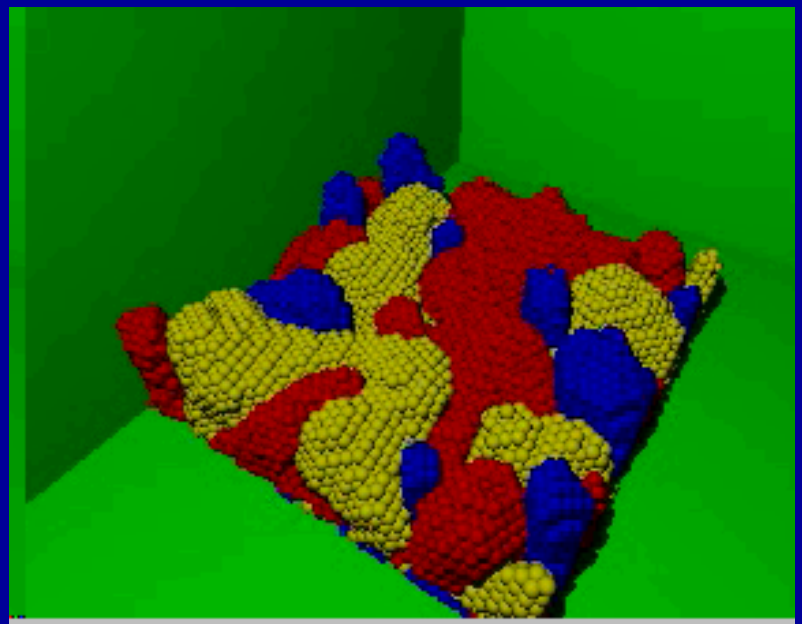
Number of atoms: 20000
Simulation size: 0.012 µm
⇒ Actual size: 0.25µm

$T_{dep} = T_{ann} = 663$ K
Annealing time = 2.7 ms



depdif30_anneal.mpg

$T_{dep} = T_{ann} = 513$ K
Annealing time = 0.18 s



depnodif10_anneal.mpg

Conclusions

- Atomistic Process Simulators provide a bridge between ab initio calculations and standard process experimental data.
- Efficient and accurate 3D simulation.
- Straighforward implementation of new mechanisms.
- Microelectronics Device Processing: “Continuum physics models are no longer sufficient below 100 nm. Tools are needed for the physical and chemical processes at an atomic level” (1997 USA National Technology Roadmap for Semiconductors)