Role of Fluctuations for Island Size Distributions during Submonolayer Epitaxy

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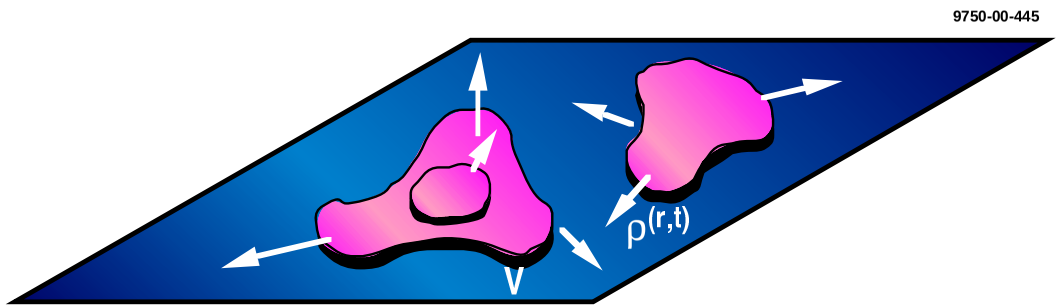
Methods Used to Study Submonolayer Epitaxy

- Rate Equations: Deterministic method
- Kinetic Monte Carlo Simulations: Stochastic method
- Possible sources of spatial and temporal fluctuations
  - Adatom concentration
  - Deposition flux
  - Nucleation of islands
  - Growth of islands
- Which fluctuations are relevant ?
- Can we construct a deterministic model ?

Island Dynamics



- Islands nucleate;
  Questions:
  - Where ?
  - When ?

- Island boundaries move
  Key quantity:
  - Velocity

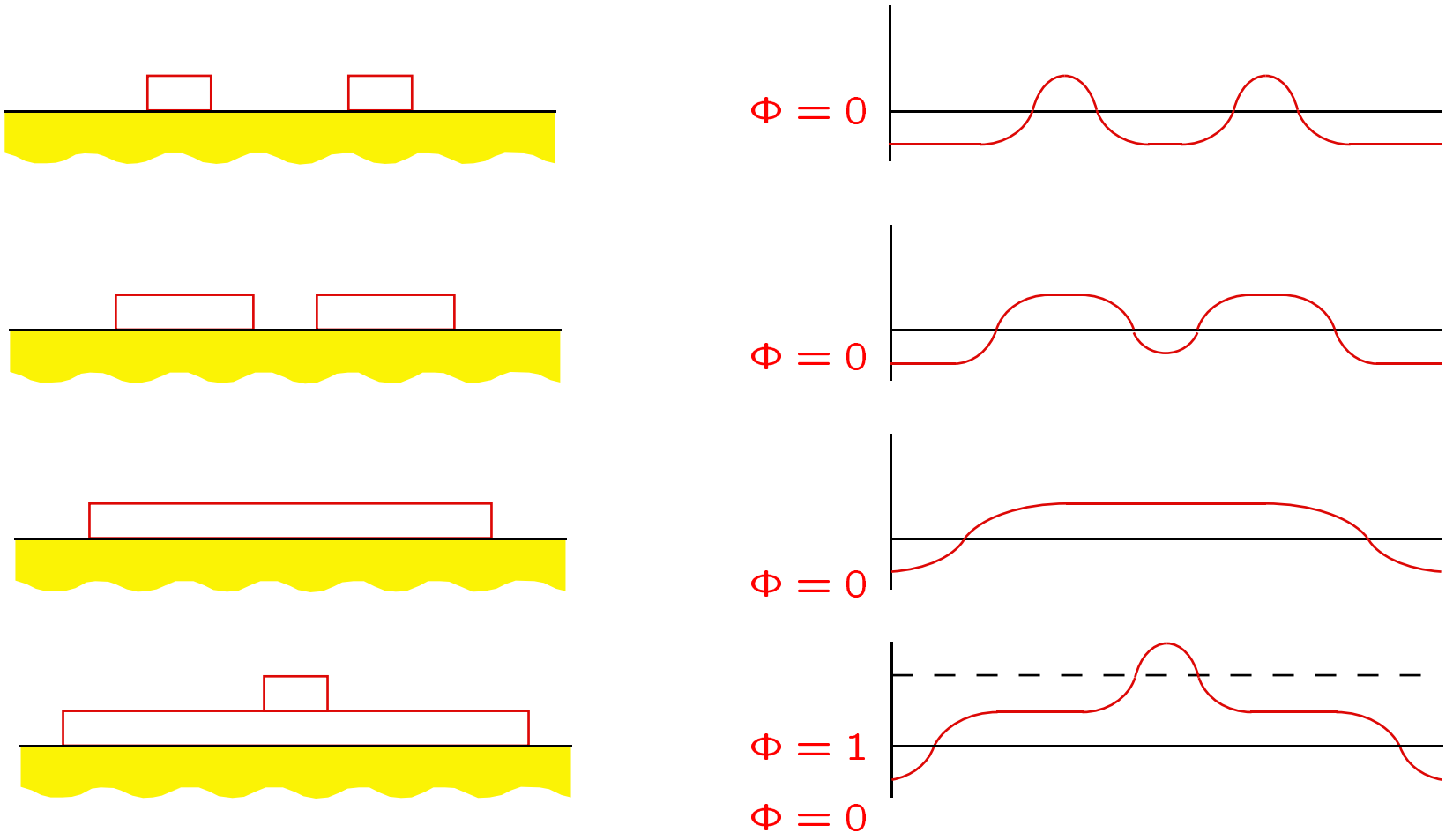
Feature size for next generation electronic devices is $\sim$ microns laterally but 10 - 100 atomic layers high.

Use Level Set Method to describe island dynamics!

The Level Set Method for Island Growth

Island Morphology

Level Set Function Φ



Governing Equation: $\frac{d\Phi}{dt} + v_n \nabla \Phi = 0$

The Model: Irreversible Aggregation

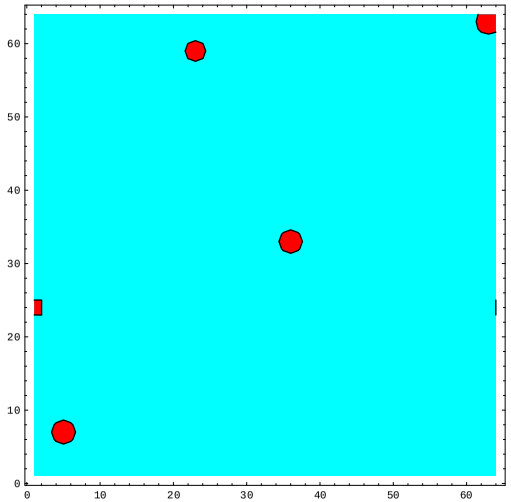
- The equation for the adatom density $\rho(\mathbf{x}, t)$ is: $\frac{d\rho}{dt} = F + D\nabla^2\rho - \frac{dN}{dt}$
- Boundary condition: $\rho = 0$ at the island boundary
- Velocity of island boundaries: $v_n = \left[D\frac{d\rho}{dn}\right]$
- Nucleation rate $\frac{dN}{dt} = D\langle\rho(\mathbf{x}, t)^2\rangle$ Determinstic in time !

But we need to decide where to seed !

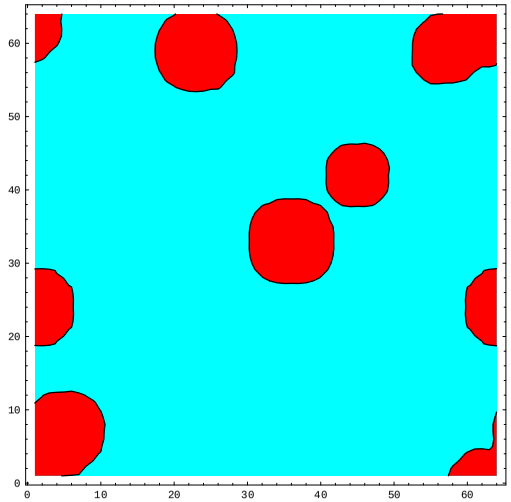
Nucleation with Spatially Varying Adatom Density

Probabilistic Island Seeding

$$\frac{dN}{dt} = C_0 \langle \rho^2 \rangle$$



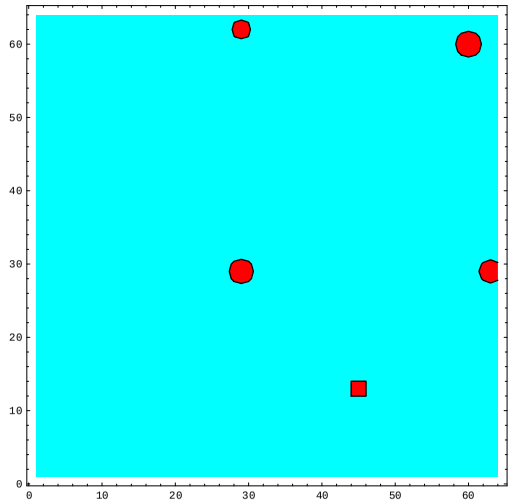
t_1

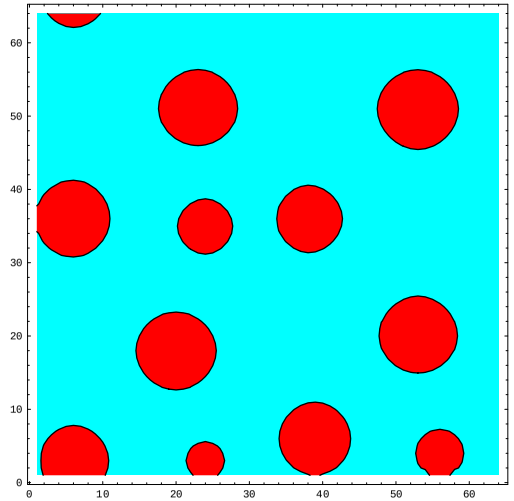


t_2

Deterministic Island Seeding

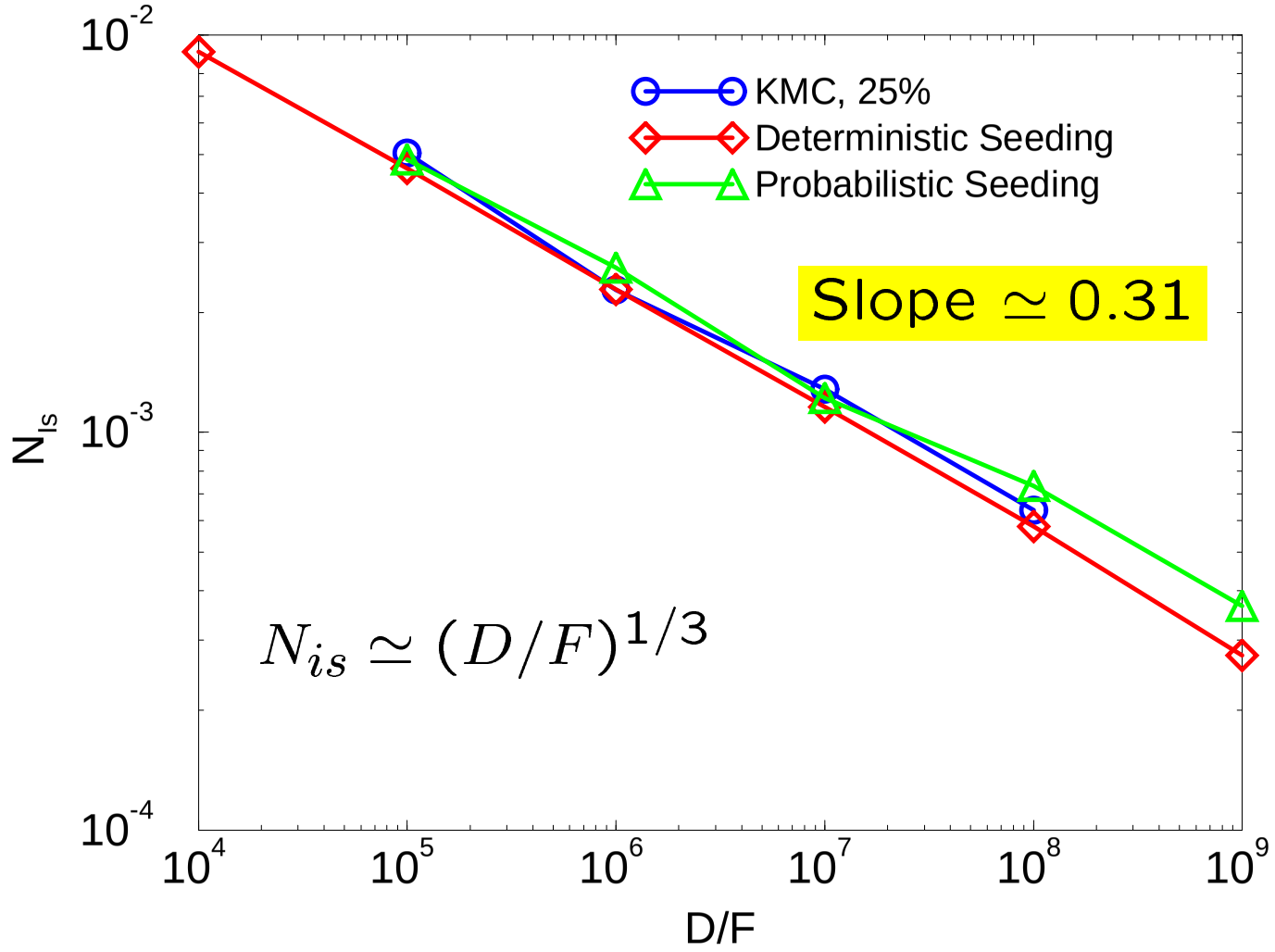
Seed at most probable point



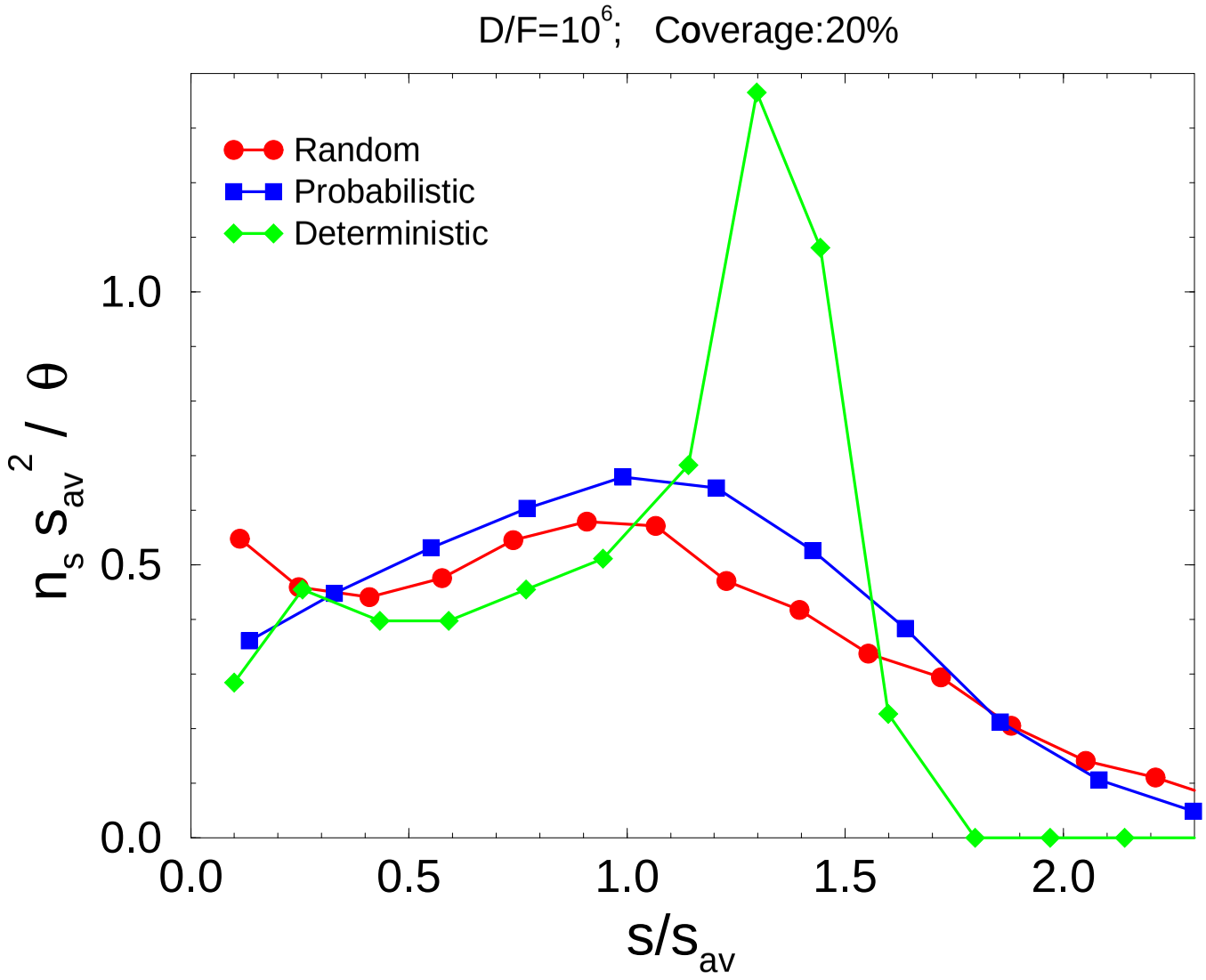


Comparison with Kinetic Monte Carlo Simulations

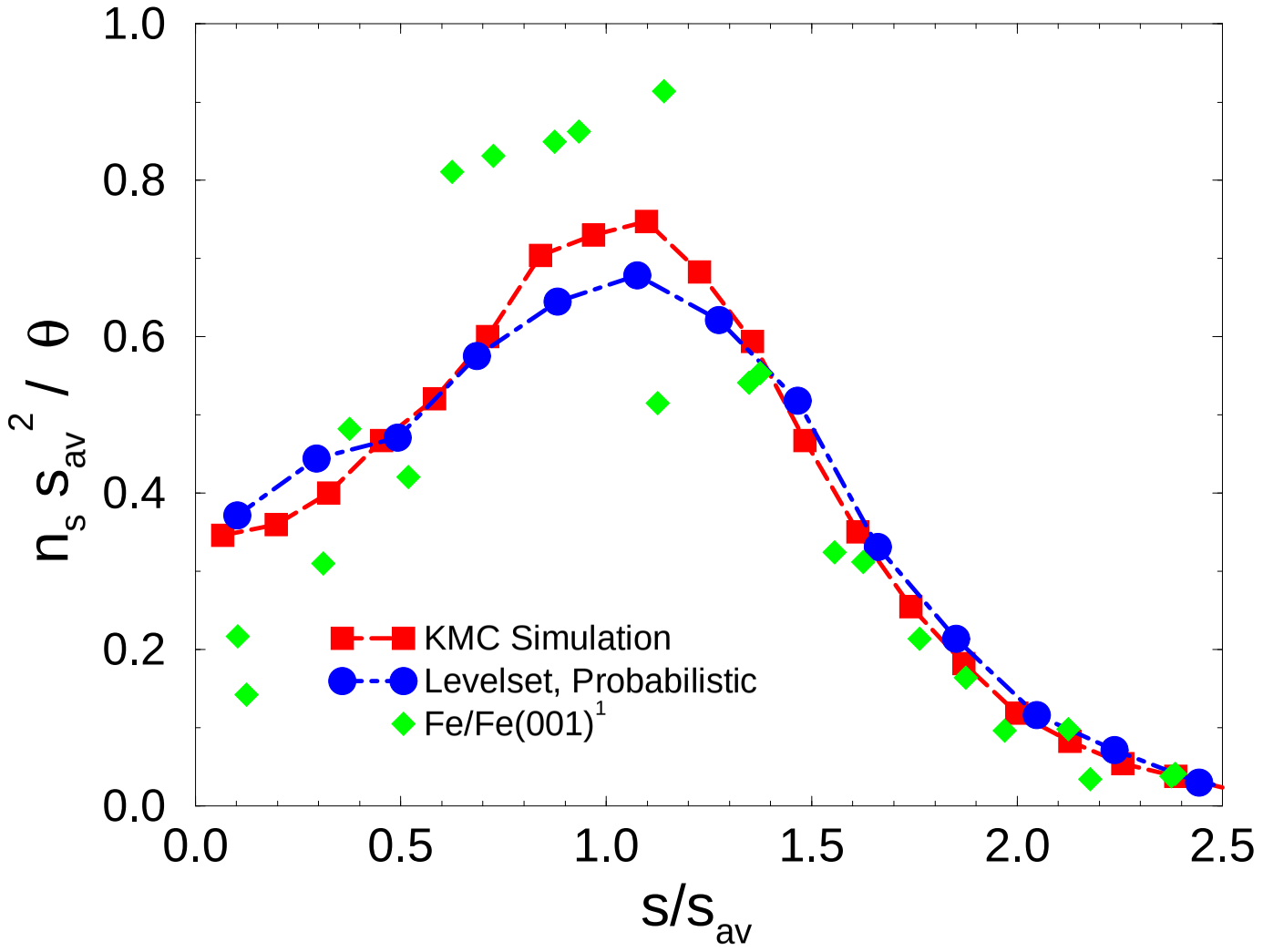
Kinetic Monte Carlo Simulation with irreversible aggregation and fast edge diffusion



Effect of Seeding Style



Probabilistic Seeding vs. KMC and Experiment

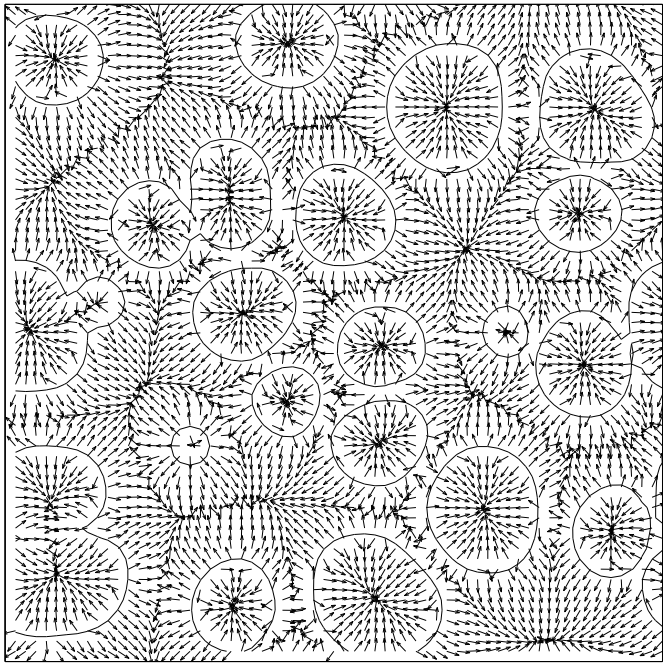


[1] J.A. Stroscio et al., PRB **46**, 1992

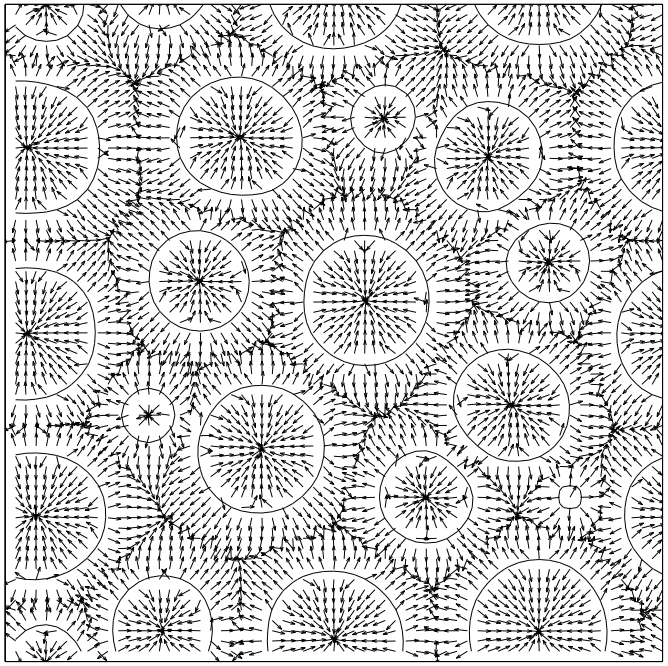
Capture Zones

The direction of the gradient of ρ gives us naturally the capture zones of islands, visualized in the following vectorplots:

Probabilistic Seeding

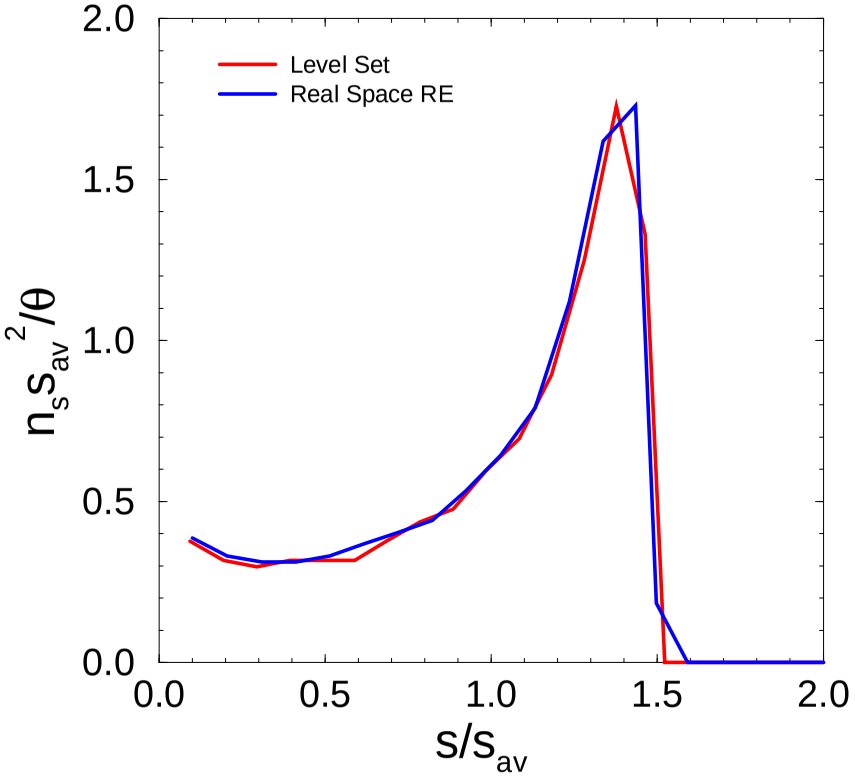


Deterministic Seeding

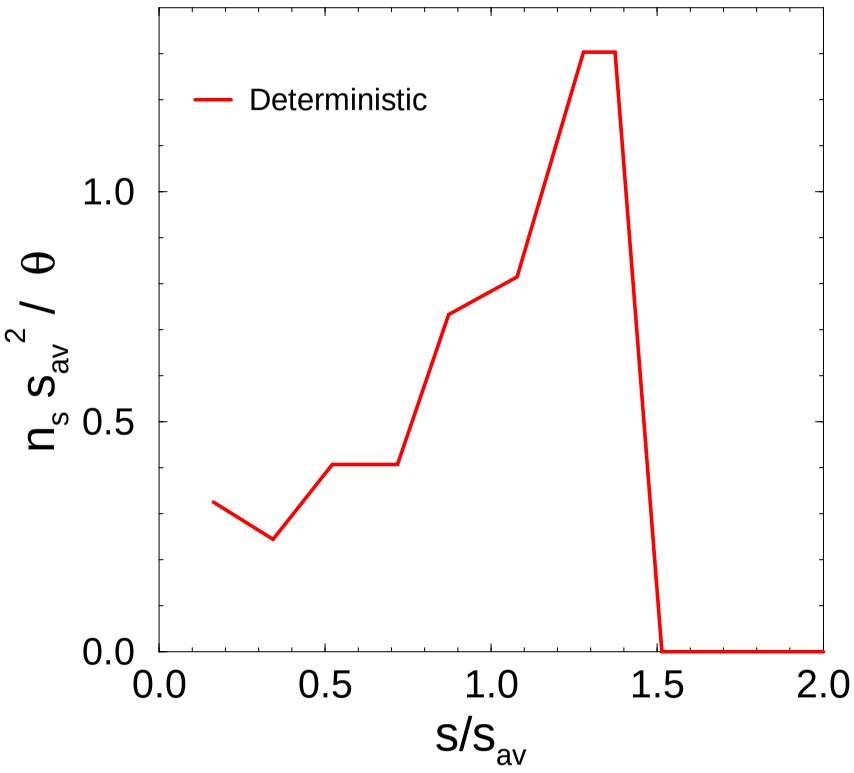


Comparison of Different Models

Model with Homogeneous adatom concentration ρ



Inhomogeneous ρ Deterministic Seeding



Model with a uniform adatom density (no spatial information) produces an island size distribution that is qualitatively similar to one obtained from a model with maximal spatial correlation.

Conclusions

- We developed a numerically stable and accurate level set method to study epitaxial growth
- We can isolate and study the effect of fluctuations during epitaxy
- Comparison with KMC-simulations shows that
  - spatial fluctuations are needed in the nucleation of islands
  - deterministic evolution of the island boundaries is appropriate
- This method provides a natural framework to couple other external fields such as strain or hydrodynamics to the growth modeling.
- The transparencies of this talk can be downloaded from http://www.math.ucla.edu/∼thinfilm/presentations/index.html