A FIRST PASSAGE TIME ALGORITHM FOR REACTION-DIFFUSION PROCESSES ON A 2D LATTICE

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Electrochemical Systems

- Chips, Batteries, Solar Cells, Fuel Cells, high density storage devices, ...
- Tremendous potential
- Important to capture fine-scale features of the deposit
Reaction-Diffusion and Nucleation
(plus attachment and growth)

Influx rate $F$

Surface Diffusivity $D$
CPU Cost for KMC simulations

From Experiments: \[ N \sim \left( \frac{D}{F} \right)^{-1} \quad \Rightarrow \quad \text{CPU time} \sim \left( \frac{D}{F} \right) \]
Diffusion over Long Distances

# steps: 100
Diffusion over Long Distances

# steps: 12300
Diffusion over Long Distances

# steps: 16200
Diffusion over Long Distances

# steps: 20300
Diffusion over Long Distances

# steps: 24300
ELFPT Algorithm: FPT on an Electronic Lattice

- Construct a protection zone around each adatom where it is guaranteed not to collide with other adatoms or bump into an island of deposit.

- Islands of deposit
- Sites where adatoms can attach to edges
- Diffusing adatoms
- Zone boundaries

First Passage Time algorithm: Oppelstrup 2006, 2009
First-Passage Time CDF Formula

- Derived formula for First-Passage Time CDF
- Derived formula for FPT location
- Exact and efficient
- Details in paper in revision, J. Comp. Phys.

\[
F(t) = P_{-L}(t) + P_{L}(t) \\
= 2 \left( 1 + \sum_{i=1}^{L} \frac{\exp \left( \lambda_{2i-1} \frac{u}{2} t \right) + 1}{\lambda_{2i-1} \prod_{j=1, j \neq i}^{L} (\lambda_{2i-1} - \lambda_{2j-1})} \right)
\]
Comparison with KMC

- Setup:
  - No edge diffusion
  - D/F varied
  - Domain Size NX varied
  - Compare CPU time to 5% coverage with deposits
Effect of D/F and Edge Diffusion
Simulation Snapshots

- Exclusion zone becomes apparent at $D/F = 10^4$
Recent Advances

- Triangular lattice
  - Physical lattices are often hexagonal densest packed (hdp), not cubic
  - So far no success deriving a closed formula for FPT
  - Pre-calculate FPT and location distributions

- Multi-Layer deposition
  - Possibility to deposit on top of already deposited material
  - Bi-Material simulation with different diffusivities on substrate and deposit

- Fast Edge Diffusion using 1D FPT
  - Was not included in previous results

- Alloy Deposition
  - Two different materials deposit on surface
  - Study chemical composition distributions of islands
Current Projects

**Silver Deposition Onto Silver (Homoepitaxy)**
- Collaboration with Dr. Ludwig Kibler (University of Ulm), estimate diffusion rates

**Silver Deposition Onto Silicon (Heteroepitaxy)**
- Collaboration with Dr. Giovanni Zangari (University of Virginia), determine grain size distributions

**Single Crystal Growth in Nano-Pipettes**
- Collaboration with Dr. Takayuki Homma (Waseda University), optimal conditions to grow a single crystal for next-gen high density storage devices
Conclusion

- New ELFPT algorithm for simulation of nucleation and growth on electronic lattice
- Speedup > 100x over KMC
- Exact algorithm: Atomic scale accuracy is maintained
- Ongoing work on electrodeposition applications
- Potential for extension to simulate wide range of surface processes
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