Acceleration of Kinetic Monte Carlo Simulation of Thin Film Deposition

Lau Yang Hao, Bharathi Madurai Srinivasan, Wu Gang, Leong Fong Yew, Ramanarayan Hariharaputran
Email: lauyh@ihpc.a-star.edu.sg

Microstructure modelling of films can be used to improve film properties

Such polycrystalline film properties, which are sensitive to microstructure, include:

Interconnect Lifetimes

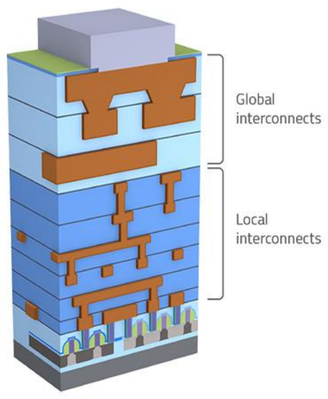
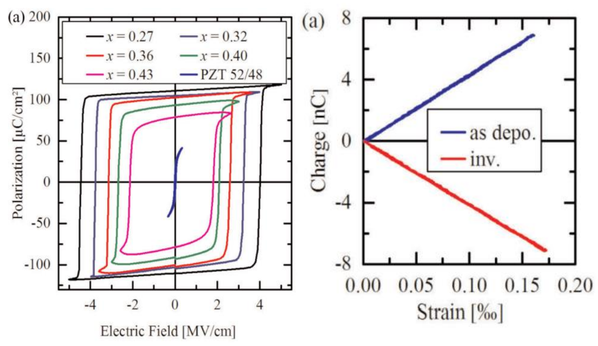


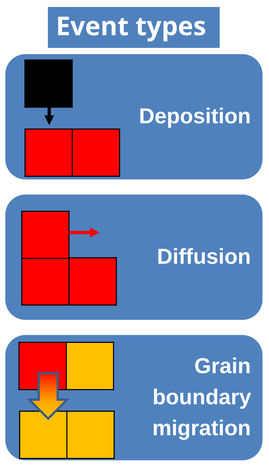
Image: Semiconduction Engineering – All about Interconnects.

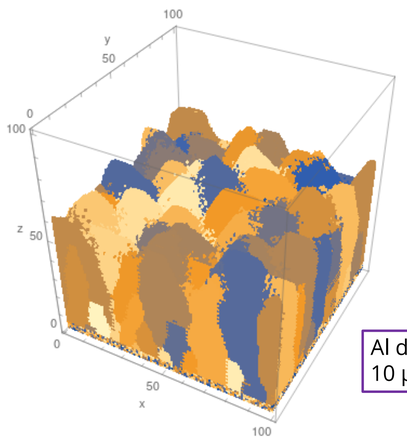
Ferroelectric and Piezoelectric Response



S. Fichtner et al., "AlScN: A III-V semiconductor based ferroelectric", Journal of Applied Physics 125, 114103 (2019).

Single-lattice Ising polycrystal (SLIP) model represents each grain as comprising atoms with the same orientation

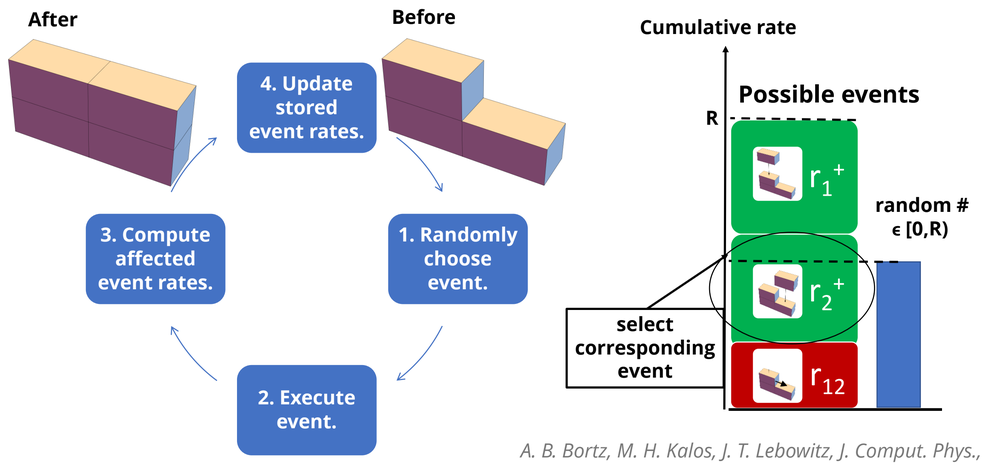




Al deposited at 10 μm/s at 300K.

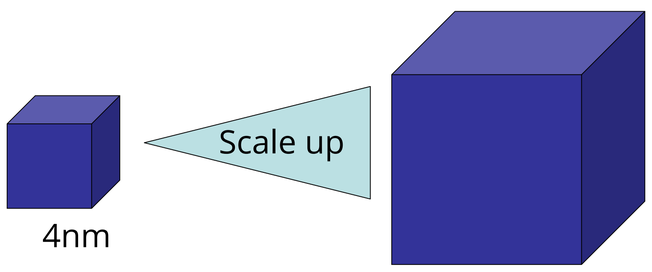
H. Huang, G.H. Gilmer, T.D. Rubia J. Appl. Phys. 84,3636 (1998).

Kinetic Monte Carlo (KMC) algorithm for SLIP simulation



A. B. Bortz, M. H. Kalos, J. T. Lebowitz, J. Comput. Phys., 17, 10 (1975).

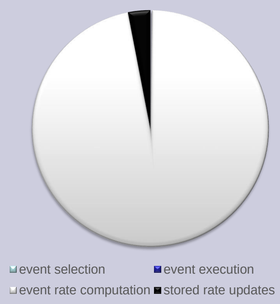
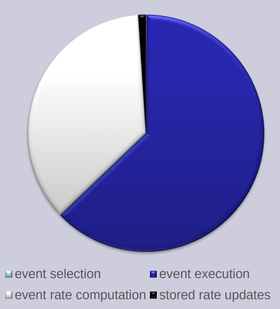
Simulating deposition of typical films takes too long



Al deposited at 10 μm/s at 300K. Runtime = 140min.

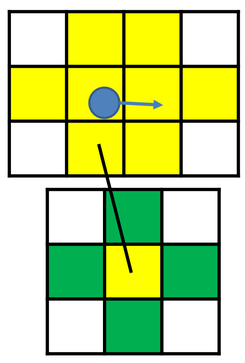
Estimated runtime = 10^3 x140min ~ 100 days.

Optimise steps where simulation spends most time

300K	0K (only deposition)
runtime: 140min	runtime: 4s
	
Most time is spent on event rate computation.	Most time is spent on event execution.

Accelerate computation of modified hop rates by incrementally updating atom energies

The hop rate depends on the energies of atoms in neighbour yellow sites.



Original algorithm

Computing hop rate by computing atom energies this way requires $O(n^2)$ steps.

Computing atom energy by looping over all n neighbors requires O(n) steps.

Accelerated version

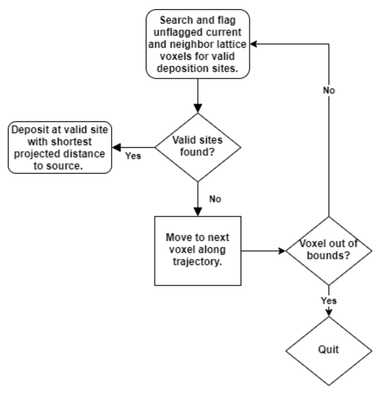
Since atom energies need not be computed, computing hop rate needs only O(n) steps.

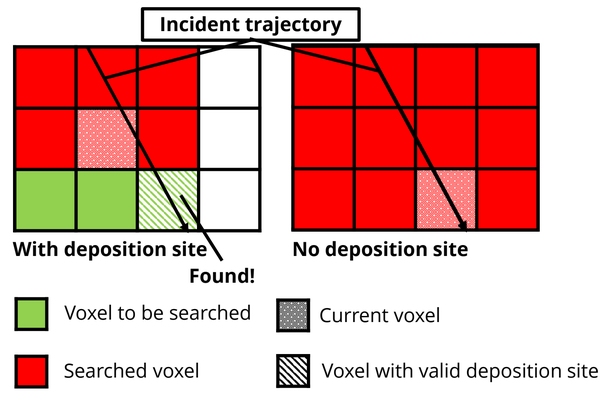
Store and update atom energies after each event with O(n) steps by looping over neighbors.

Energy of the atom in the yellow site depends on coordination and misorientation with atoms in the neighbouring green sites.

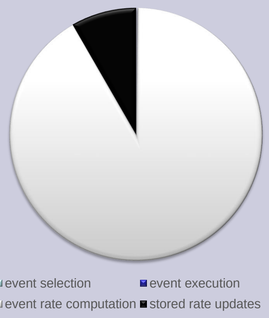
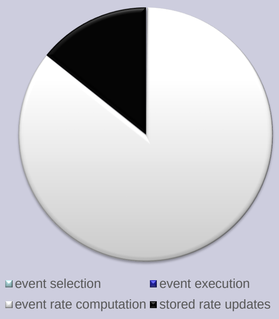
Accelerate deposition by searching for deposition site only along incident trajectory

- For every deposition, original program checks every one of N lattice sites to obtain valid deposition sites.
- Only sites along trajectory, numbering $O(\sqrt[3]{N})$, need to be checked.
- To handle arbitrary site distributions, accelerated version stores sites in cubic lattice with spacing = capture distance.
- Starting from particle source above film,

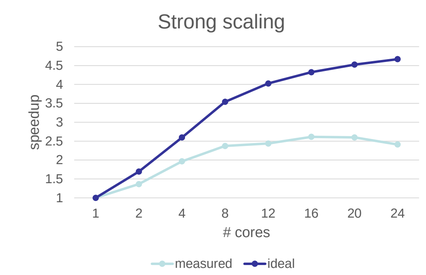


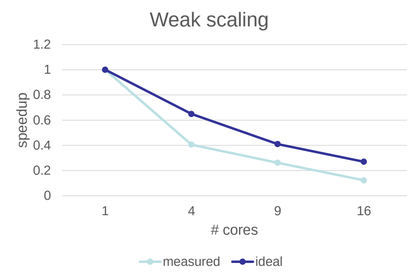


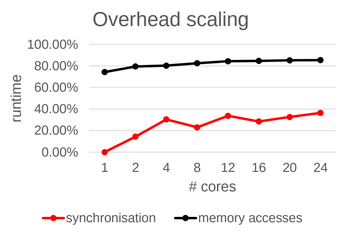
Optimisations accelerate simulation by alleviating rate limiting steps

300K	0K
4.8x speedup	2x speedup
	
Less time is spent on event rate computation.	Less time is spent on event execution.

Distribute computation of different event rates to different cores using openMP to achieve further speedup







Less-than-ideal scaling due to synchronisation overhead and increased memory use.

Better scaling from further memory optimisation possible.

Conclusions

1. Incremental atom energy updates.	Reduces complexity of hop rate computation from $O(n^2)$ to $O(n)$.
2. Searching only around incident atom trajectories.	Reduces complexity of finding deposition sites from $O(N)$ to $O(\sqrt[3]{N})$.
4.8x speedup	

Parallelisation of event rate computation.

2.6x max speedup

12x net max speedup

Accelerated code may guide manufacturing process to optimise film quality.

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