Acceleration of Kinetic Monte Carlo simulation of thin film deposition

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Kinetic Monte Carlo (KMC) is faster than molecular dynamics and can therefore reach larger time and length scales. As such, KMC lends itself well to studying the effects of stochastic processes like nucleation, diffusion, and coarsening on the microstructure of materials. As these processes often occur during deposition or annealing of thin films, which are widely used as, e.g., electronic semiconductor devices and optical coating, KMC has been used to simulate the evolution of film microstructure and investigate how said microstructure depends on processing conditions. Doing so for typical sizes of manufactured films often requires excessive computational times, making it impossible to realize the dream of solving the inverse process-microstructure problem in a timely manner, by conducting many high throughput simulations to rapidly explore the phase space of process conditions to determine optimal conditions to achieve a desired microstructure. As such, various strategies have been employed to accelerate such simulations.

These strategies can be broadly classed as either spatial parallelization or coarse graining. The former tends to result in inefficient algorithms as KMC is inherently asynchronous. This synchronization overhead is mitigated in the synchronous sub-lattice parallelization scheme, but the algorithm is only semi rigorous. Another approach is to perfectly synchronize domains by using the same time step in each CPU, but removing the random variation between time steps taken by each CPU also has an unclear impact on simulation accuracy. Due to its inefficiency or inaccuracy, parallelization of KMC is rarely employed.

In practice, coarse graining is more often used. Coarse graining space, groups of atoms, or events increases the physical time each simulation step covers, thus allowing processes to be simulated with fewer steps. However, the resulting speedup comes at a cost - reduced resolution and often accuracy when simplifying approximations are made.

Because of the uncertainty or inefficiency surrounding spatial parallelization and coarse graining, it is safer to stick with and optimize the original algorithm while retaining fidelity of its output. To do so, we follow the usual approach of profiling the simulation to find and mitigate bottlenecks. The simulation we use as demonstration of our acceleration scheme implements the well studied Single Lattice Ising Polycrystal (SLIP) model [2], through extension of the SPPARKS KMC simulator (https://spparks.github.io/index.html) [1]. A typical simulation result is shown in Figure 1. After determining the simulation spends most run-time computing event rates, we apply various optimizations to minimize and accelerate, as well as parallelize, such computations. Since such computations make up the majority of the simulation time, Amdahl's law predicts an ideal parallel speedup close to the number of cores used.

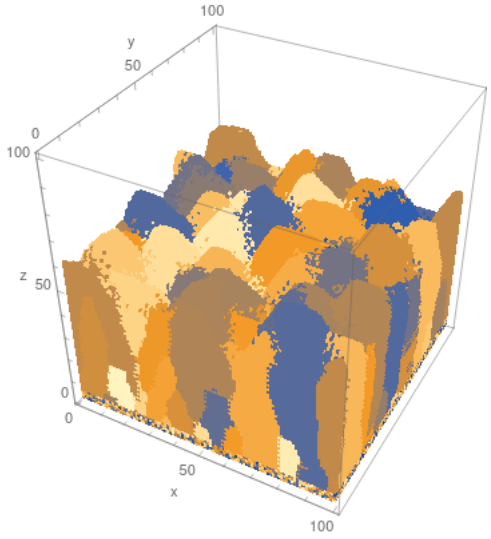

Figure 1: Microstructure of Al deposited at 300K at 10 microns per second. Different colors indicate different grain orientations.

We measure the impact of these acceleration strategies on runtime and show how they scale with number of cores. The accelerated code allows simulation of larger domains over longer durations, approaching the scales necessary to guide the manufacturing process to optimize film quality.

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