An Efficient Atomistic Method for Micro-Scale Film Growth from the Vapor Phase

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We present a multi-scale method for the simulation of vapor deposition processes in micrometer-sized structures with full atomistic representation. Our method couples Kinetic Monte Carlo (KMC) sampling at the microscale with Molecular Dynamics (MD) simulations at the nanoscale. Parallel efficiency is improved through a maintainable active surface graph representation, which accelerates the search for adsorption sites and enables seamless subdomains for MD simulations. The surrounding gas phase and growing surfaces are modeled geometrically and linked to the presented method.

Coupling Method: Fig. 1 shows the coupling method of the atomistic deposition model. Adsorption events are sampled using KMC methods at the active surface. Selected events are simulated using MD in subdomains around the adsorption site. After each event, the atoms are frozen and reinserted in-place into the global domain, and the active surface and the event candidates are updated. Seamless reinsertion is guaranteed through a shared boundary region between the domains.

KMC Adsorption Sampling: A direct method KMC algorithm is used to sample adsorption events with overestimating rate heuristics at the active surface. Since KMC is inherently sequential and MD simulations take some seconds to complete, placeholder Null events and limited time warping are used to evaluate events in parallel while preserving the system's KMC dynamics.

MD Adsorption Simulations: Each adsorption event is evaluated with an explicit LAMMPS MD simulation in a local subdomain around the adsorption site. The incident atom is placed above the adsorption site, with a velocity according to the process characteristics, and a NVE simulation with a bulk-only thermostat is performed. This allows for the accurate modelling of the adsorption process, and yields film morphologies from MD force fields.

Surface Representation: An Alpha Shape representation of the growing surface is used as an acceleration structure for KMC candidate searches. The Alpha Shape is constructed from the Delaunay triangulation of the atom positions by omission of tetrahedra with circumradii $r_{\mathrm{circ}}>\alpha$. Since this criterion limits the influence of each atom to a radius of 2α, the Alpha Shape construction can be performed in space-filling subdomains with overlapping boundaries of size 2α. This enables the seamless local update of the Alpha Shape after each MD simulation without the need for computationally expensive global re-triangulations.

Particle Transport in the Gas Phase: To incorporate gas phase particle transport and surfaces surrounding the atomistic region, the presented deposition model is linked to a geometric particle transport model in the free molecular flow regime. Particles are traced linearly between surfaces, and precomputed particle-surface interaction statistics are applied. Non-atomistic surrounding surfaces are modeled with a geometric surface growth model. Through the use of modern raytracing techniques and hardware acceleration, the surface sampling resolution from incident gas particles is improved.

Geometric Surface Growth: A Level Set method is used to represent the surrounding growing surface as a scalar field, and advance the surface according to the local growth rates as calculated from the particle-surface interactions, as shown in Fig. 2. Incident particle statistics for the atomistic method is then sampled in predefined surface regions.

References

[1] J. Gehre, *Coupling between stochastic particle transport models and topographic thin film growth*, Master Thesis, TU Chemnitz (2022). https://nbn-resolving.org/urn:nbn:de:bsz:ch1-qucosa2-786436

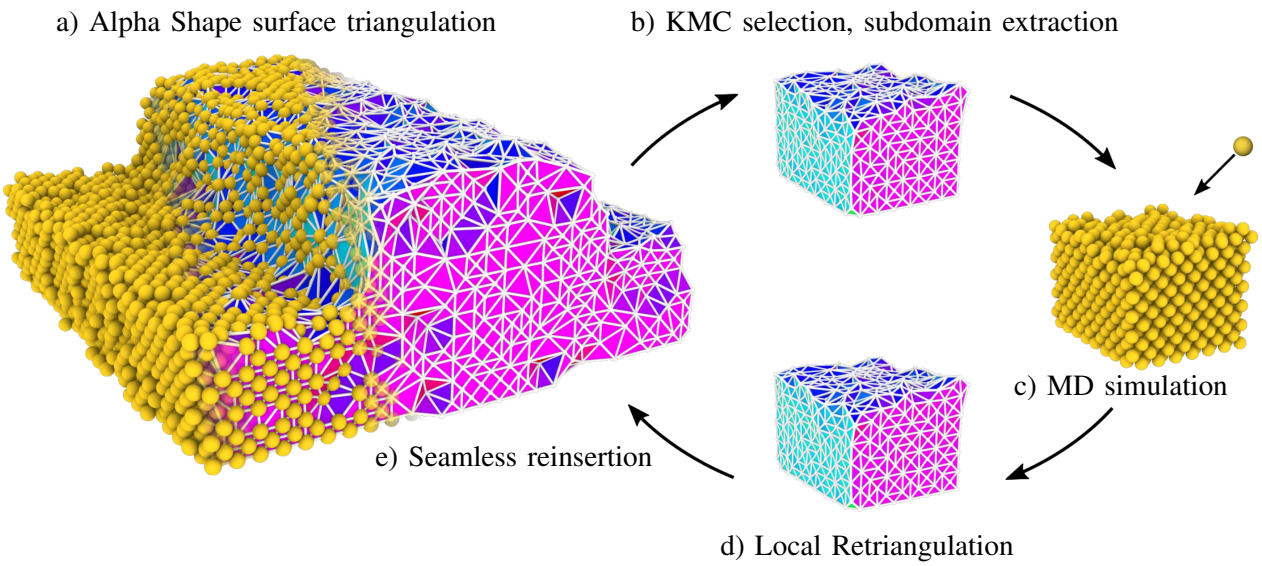

Fig. 1. Circular coupling method of the atomistic vapor deposition model: a) Global triangulation and Alpha Shape construction of the active surface b) KMC sampling of adsorption events at the active surface c) MD simulation around the adsorption site d) Local retriangulation of the subdomain e) Seamless reinsertion due to a shared domain boundary and the alpha criterion

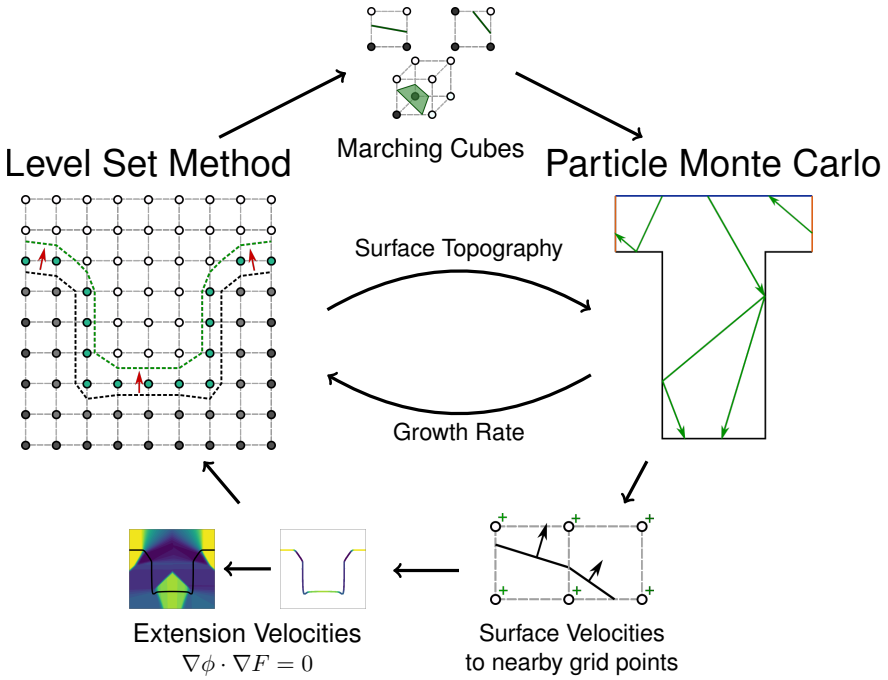

Fig. 2. Geomectric surface growth model: Surface is maintained in the Level Set representation, and is advanced according to the local growth rate sampled from particle Monte Carlo simulations.