

# QUASI-EQUILIBRIUM OFF-LATTICE KINETIC MONTE CARLO

HENRY BOATENG, UNIVERSITY OF MICHIGAN

We present an off-lattice kinetic Monte Carlo algorithm in  $(1+1)$ -dimensions that drives surface diffusion by a chemical potential gradient. Interactions between atoms are defined by the Lennard-Jones potential which removes the restriction on atomic positions to lattice points enforced by lattice based models. The method is validated by simulations of hetero-epitaxial growth, annealing of strained bilayer systems and a qualitative verification of Stoney's formula. The algorithm captures the effect of misfit and deposition flux on island formation, the formation of vacancies and edge dislocations unlike lattice and continuum models, and naturally incorporates intermixing.