Exercise 2: MC simulations of Ag growth

We model growth on the (001) Ag surface using a $h(x,y)$ solid-on-solid representation on a square lattice. A $L \times L = 60 \times 60$ periodic cell is considered, unless differently indicated. Atomic interactions are limited to first-neighbors only, with bonding energy $J_1 = -0.345 \, eV$. Each Ag atom is bonded to 4 neighbors from the underlying layer, i.e. $J_0 = 4J_1$, and can form up to 4 lateral bonds (each of energy J_1) with atoms in adjacent columns.

PART A: kinetic Monte-Carlo

Implement a Kinetic Monte-Carlo code to simulate Ag epitaxy starting from a flat surface $h(x,y) = 0$. Deposition occurs with a uniform rate ϕ. Topmost surface atoms can hop on top of any of the 4 nearest-neighbor atomic columns with identical probability. The diffusion rate is set with attempt frequency $\nu = 10^{13} \, Hz$ and activation barrier given by bond counting as $E_b = -(J_0 + n_1 J_1)$.

Nominal coverage (number of deposited layers): $\theta = \phi t$.

RMS roughness: $\sigma = \sqrt{\langle h^2 \rangle - \langle h \rangle^2}$.

1. Perform a simulation of deposition only ($0 \, K$, i.e. no diffusion) with $\phi = 0.2 \, ML/s$ up to a nominal coverage $\theta = 5 \, ML$. Analyze the sequence of escape times τ extracted for each deposition event and test that their average corresponds to the reciprocal of total deposition rate and check that τ values distribute with the expected exponential distribution. Observe the morphology of the deposited film and the square-root behavior of $\sigma(\theta)$.

2. Perform growth simulations at $T = 650 \, K$ with deposition flux $\phi = [10, \, 1, \, 0.1, \, 0.01, 0.0001] \, ML/s$, up to a nominal thickness of $\theta = 5 \, ML$. Observe the different growth modes and compare the behavior of $\sigma(\theta)$. In the cases corresponding to layer-by-layer growth, what is the effect of decreasing ϕ (look at the early stages, e.g. after deposition of $0.1 \, ML$)? Interpret the results. If the growth apparatus only works at $\phi = 1 \, ML/s$, is it possible to achieve the same behavior previously observed for $\phi = 0.01 \, ML/s$ by tuning the temperature?