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?

PART B: Metropolis MC

Implement a Metropolis MC loop to find the equilibrium configuration of a Ag cluster of fixed number of atoms N, randomly deposited on the flat $h(x,y) = 0$ substrate. The energy of each configuration is evaluated by counting all bonds, (energies J_0 and J_1) formed by the N atoms above the substrate. Each MC move consists in relocating one adatom at a randomly chosen site.

1. Consider the MC loop at $T = 0\ K$ and find the minimum-energy configuration of clusters from $N = 2$ to 20. Check that in each case the global minimum is found by considering a long-enough MC loop and avoid metastable configurations by changing the random generator seed. Plot the energy of the minima $E_{min}(N)$ and the chemical potential $\mu(N) = E_{min}(N)/N$. Analyze the results and interpret the alternating slope of $\mu(N)$ by considering the changes from one configuration to the next.

2. Study the equilibrium configuration of the $N = 25$ cluster as a function of temperature, in the range $1 - 2700\ K$. For each simulation compute the average energy $\langle E \rangle$ and standard deviation $\Sigma = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$ at equilibrium (find the appropriate number of MC steps to be excluded as corresponding to thermalization and run the loop long enough to have a sufficient number of configurations to obtain meaningful averages). Check robustness by repeating the calculation for different seeds. Plot $\langle E \rangle(T)$ and $\Sigma(T)$ (select a convenient set of T values to trace smooth curves). Repeat the analysis for $L = 40$ and $L = 20$ and compare the $\langle E \rangle(T)$ and $\Sigma(T)$ curves. Interpret the result.