Kinetic Monte Carlo Simulation of Al Diffusion in Cu

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1. Kinetic Monte Carlo Algorithm

The Kinetic Monte Carlo (KMC) algorithm simulates atomic-scale diffusion processes using stochastic methods. It is particularly effective for capturing time evolution in systems where rare events dominate, such as atomistic diffusion.

Figure 1 illustrates the complete KMC simulation flowchart. The key steps are:

1. **Initialization:** A 2D lattice is created, and Al atoms are distributed in the lower half with a predefined concentration.
2. **Physics setup:** The temperature-dependent diffusion coefficient D is computed using the Arrhenius relation. Based on D, the atomic jump frequency ν is calculated.
3. **Main KMC Loop:** For each time step:
   - All valid Al jumps are identified (i.e., moves to empty neighboring sites).
   - A total transition rate Γ is computed from the individual rates.
   - A jump is selected probabilistically using a random number R_1.
   - The jump is executed and the lattice is updated.
   - A second random number R_2 is used to compute the time increment Δt.
   - Simulation time is updated and the loop continues until the termination condition is met.
4. **Termination:** When the total simulation time exceeds a predefined limit or a maximum number of steps is reached, the simulation ends and the final Al distribution is output.

Boundary conditions: Periodic boundaries are applied along the horizontal (in-plane) directions. An atom can only move to a neighboring site if it is unoccupied (i.e., not blocked).

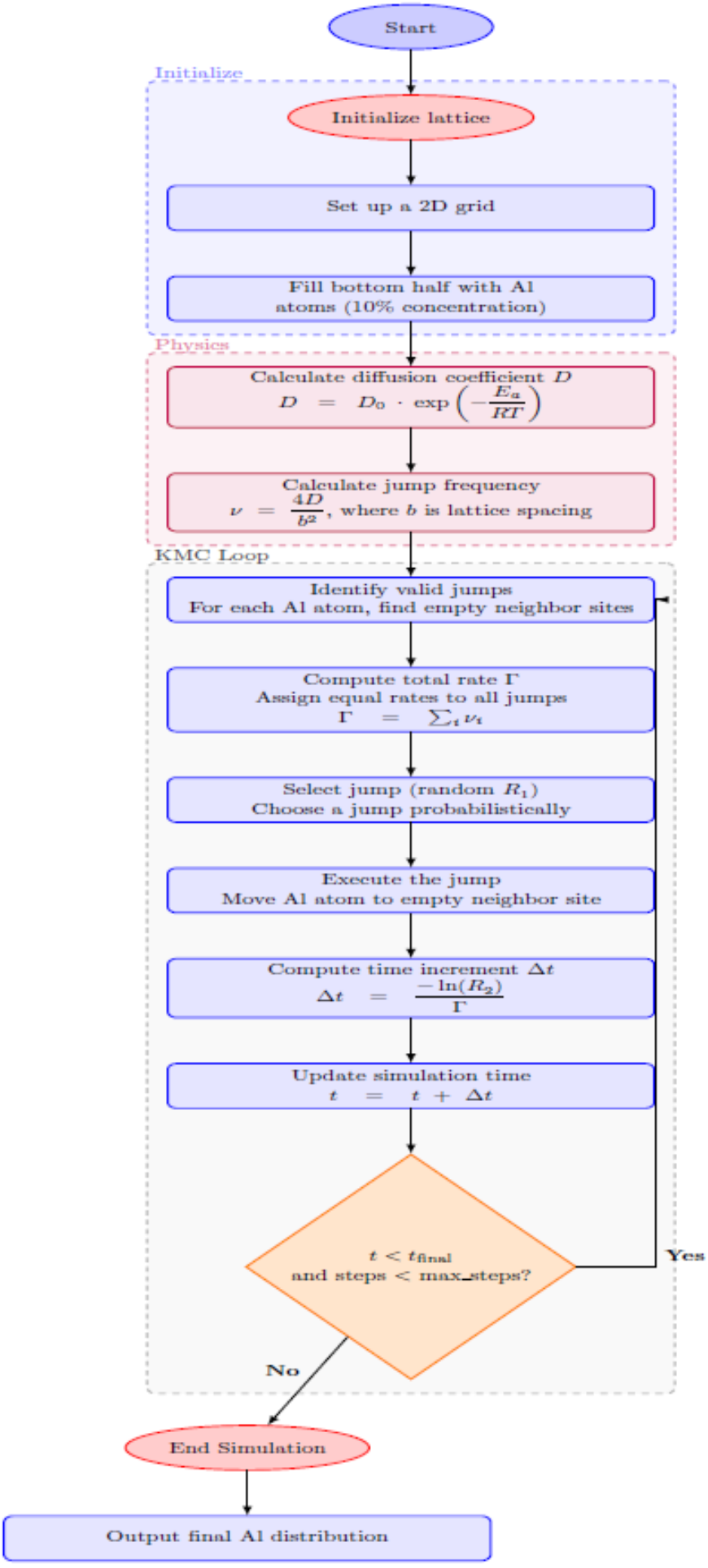

Figure 1: KMC algorithm flowchart

2. Diffusion Coefficient and Rate Relation

The temperature-dependent diffusion coefficient $D(T)$ is given by:

$$D(T) = D_0 \cdot \exp\left(-\frac{E_a}{RT}\right)$$

The corresponding microscopic jump rate is:

$$\nu = \frac{4D}{b^2}$$

with $b = 2.54 \times 10^{-10}\,\text{m}$, $D_0 = 1.49 \times 10^{-7}\,\text{m}^2/\text{s}$, and $E_a = 137.1\,\text{kJ/mol}$.

3. Simulation Results at Constant Temperatures

The following figure shows the KMC simulation results at 500K and 600K compared against the analytical error function solution:

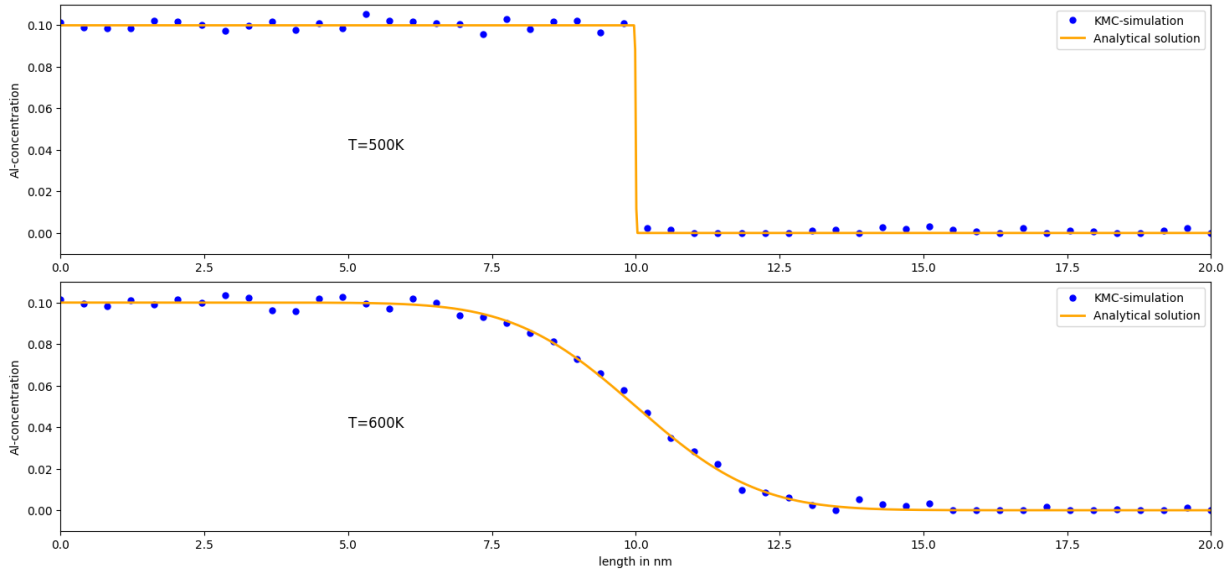

Fig. 2: Evolution of concentration profiles in a 20nm × 20nm sandwich structure at T=500K and T=600K for a time duration of 10s.

Figure 2: Comparison of Al concentration profiles from KMC and analytical solutions at constant temperatures

4. Diffusion Profile Comparison with Analytical Error Function

The 1D concentration profile from the KMC simulation is compared with the analytical error function solution. This comparison validates the consistency of the simulation at $T = 600\,K$ over a time duration of $5\,s$.

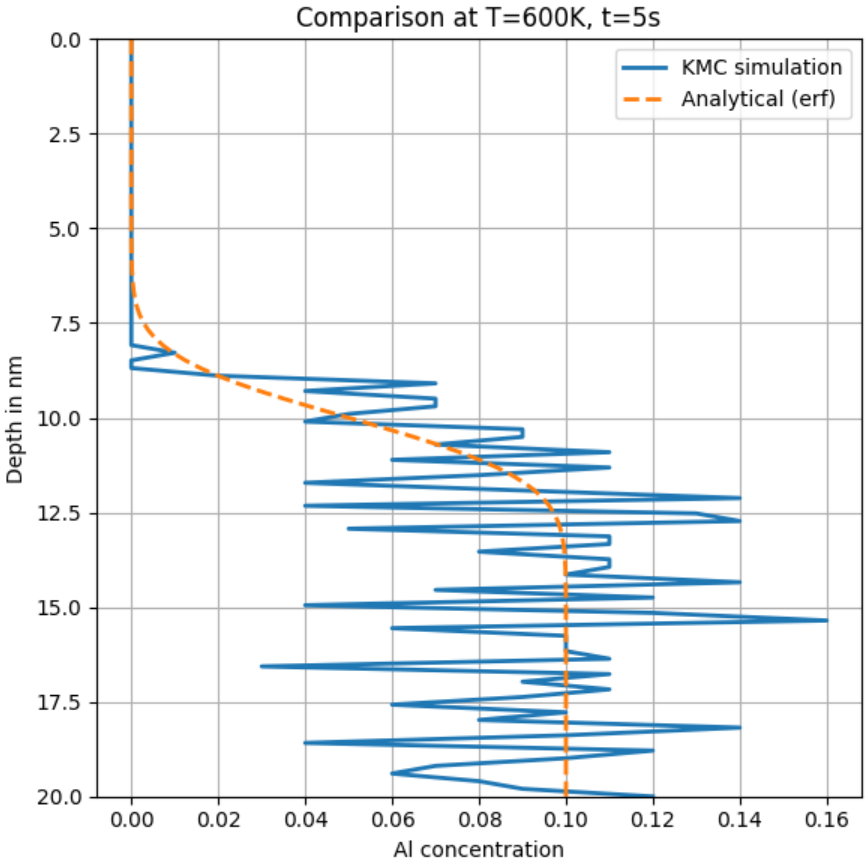

Figure 3: Diffusion profile error function solution

5. Diffusion Profile and Al Distribution

The following figure shows two aspects of the final Al distribution:

- Left: 1D average profile along film thickness (vertical).
- Right: 2D scatter plot showing spatial distribution of Al atoms.

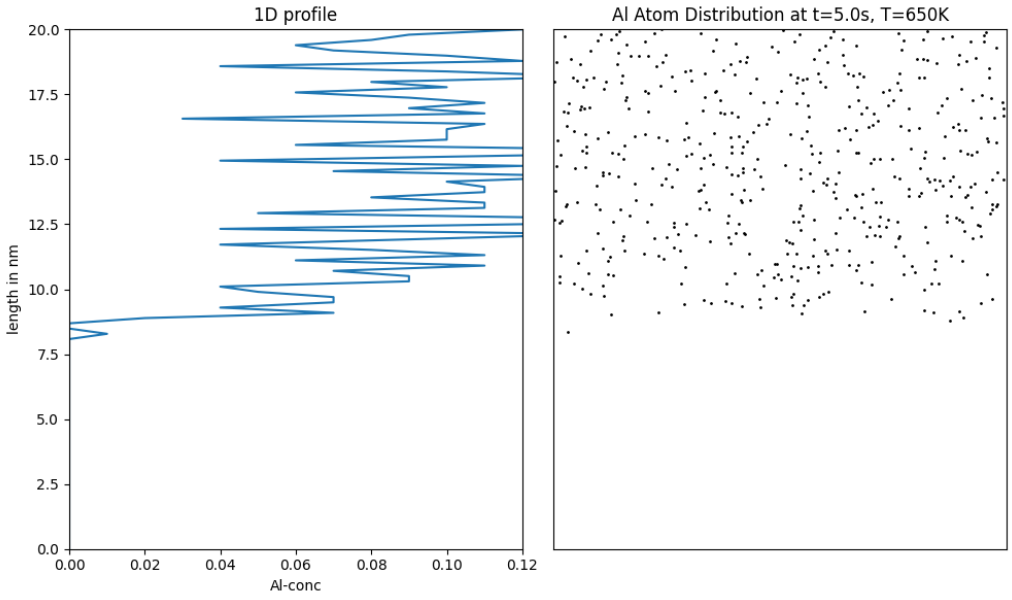

Figure 4: Final 1D and 2D Al atom distribution at $T = 650\,K$ and $t = 5\,s$

6. Coarse-Grained Simulation

In the coarse-grained model, the film is divided into cells and inter-cell transitions are computed using:

$$\frac{dC_i}{dt} = D \cdot \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2}$$

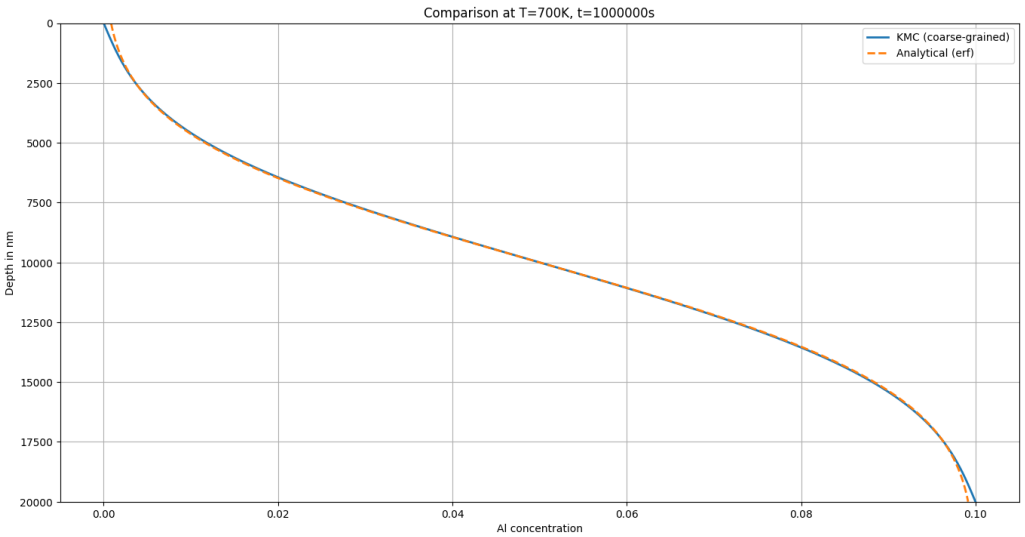

Figure 5: Time evolution of the diffuse layer using coarse-grained diffusion model

7. Observations

- KMC captures stochastic behavior of diffusion, especially at low temperatures and short times.
- At higher temperatures or longer durations, KMC closely matches analytical profiles.
- The 2D scatter plot reveals the spatial inhomogeneity and stochasticity in diffusion.
- Coarse-graining simplifies computation for large-scale, long-time simulations.