Project Progress Report: Monte Carlo Simulation of Thin Film Deposition and Growth

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Contents

1 Abstract

In the field of nanotechnology, the fabrication of materials with precisely controlled properties is of atmost importance. Thin layers of material in the range of nanometers to micrometers in thickness are building blocks for modern technologies, including semiconductor devices, optical coatings and magnetic storage media. The functionality and performance of these devices are critically dependent on the structural characteristics of the thin film, particularly its surface morphology and roughness.

The growth of a thin film is a complex, non-equilibrium process governed by the interplay of various atomic-scale events. When atoms or molecules (flux) arrive at a substrate, they can adsorb, diffuse across the surface, bond with other atoms, and even desorb. The competition between these processes dictates the final structure of the film. For example, a process dominated by random sticking with little surface movement results in a rough film, while a process allowing for significant atomic diffusion can lead to a smooth, crystalline layer.

This project employs the Monte Carlo simulation method to investigate the principles of surface growth through models representing different levels of physical complexity. The implemented models include:

1. **Random Deposition (RD):** The simplest baseline model, involving only particle adhesion (Deposition).
2. **Edwards–Wilkinson (EW):** A linear model introducing surface relaxation via diffusion, implemented in both 1D and 3D.
3. **Kardar–Parisi–Zhang (KPZ):** A non-linear model accounting for slope-dependent lateral growth, implemented in both 1D and 3D.
4. **Ballistic Deposition (BD):** A discrete model capturing geometric shadowing effects and columnar growth in 2D substrate.
5. **Kinetic Monte Carlo (KMC):** An advanced Atomistic simulation incorporating temperature-dependent diffusion, material-specific activation energies.

These models provide a comprehensive framework for understanding thin film growth from statistical mechanics to realistic, material-specific predictions.

Link to Code Base : https://github.com/shadowPunch/Monte-Carlo-simulation-of-Nanofilm-Depostion

2 Literature Review

The simulation of thin film growth has evolved through multiple generations of models, each addressing specific physical phenomena while introducing new limitations. The current literature spans from abstract continuum theories to fully atomistic methods, with trade-offs between computational tractability and material-specificity.

Continuum Models:
The Edwards-Wilkinson (EW) and Kardar-Parisi-Zhang (KPZ) equations represent the continuum approach to surface growth. These models describe surface evolution through stochastic differential equations. The EW model predicts a growth exponent of $\beta = 1/4$ in one dimension through linear surface tension-driven relaxation, while the KPZ equation introduces non-linear lateral growth effects yielding $\beta = 1/3$. However, they average over atomistic details and cannot capture material-specific chemistry.

Ballistic Deposition Models:
Discrete ballistic deposition (BD) models capture geometric shadowing effects absent from continuum theories . These models have proven particularly successful for simulating low-temperature physical vapor deposition where directional flux and limited thermal diffusion dominate. However, pure BD models completely neglect thermal surface mobility.

Kinetic Monte Carlo:
KMC employs the rare-event approximation to reach millisecond timescales by focusing computational effort on barrier-crossing events rather than thermal vibrations. Three-dimensional KMC simulations of transition metal nitrides have successfully extracted growth and roughness exponents in quantitative agreement with experimental data.

2.1 Project Contribution

This project directly addresses these gaps through:

- Development of a hierarchical simulation framework progressing from RD through EW/KPZ to ballistic deposition and finally to material-specific KMC, providing clarity on the role of each physical mechanism.
- Systematic implementation in both 1D and 2D/3D geometries, showing dimensional effects on growth exponents and morphology.
- Creation of a hybrid ballistic model that captures the realistic competition between roughening and smoothing mechanisms.
- Implementation of material-specific KMC framework where activation energies are explicit input parameters, enabling simulation of different materials without code modification.

3 Models of Surface Growth

The primary metric for characterizing a growing surface is its roughness, often defined as the root-mean-square (RMS) fluctuation of the surface height $h(\mathbf{x}, t)$. For a system of size L and dimension d, it is given by:

$$w(L,t) = \sqrt{\frac{1}{L^d}\sum_{\mathbf{x}}[h(\mathbf{x},t) - \bar{h}(t)]^2}$$

where $\bar{h}(t)$ is the average height at time t. A key insight in the study of dynamic surfaces is that this roughness often evolves according to a power law, $w(t) \propto t^\beta$, where β is the *growth exponent*. This exponent is a universal characteristic of the growth process, and different physical models predict distinct values of β.

3.1 Random Deposition (RD)

The Random Deposition model is the simplest model of surface growth. It operates on a single assumption: particles deposit at random locations on the substrate and are permanently fixed at that position. There is no diffusion, or interaction between neighboring columns. The growth of each column is independent of all others.

The number of particles in any given column follows a Poisson distribution. A fundamental property of the Poisson distribution is that its variance is equal to its mean. Since the mean height $\bar{h}(t)$ grows linearly with deposition time t, the variance of the height fluctuations, $w^2(t)$, must also be proportional to time:

$$w^2(t) \propto \bar{h}(t) \propto t$$

Taking the square root yields the scaling relation for the roughness:

$$w(t) \propto t^{1/2}$$

Thus, the RD model predicts a growth exponent of $\beta = 1/2$. While physically unrealistic for most systems, it serves as a theoretical baseline for what happens in the complete absence of any surface relaxation mechanism.

3.2 Edwards–Wilkinson (EW) Model

The EW model introduces the first crucial element of realism: surface relaxation. It recognizes that deposited atoms (adatoms) are not necessarily immobile. They possess some surface mobility and will tend to move towards positions of lower energy, which typically correspond to sites with more neighbors. This process is analogous to surface tension in a fluid, which acts to minimize surface area and smooth out fluctuations.

The rate of change of the height is described by:

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu\nabla^2 h(\mathbf{x},t) + \eta(\mathbf{x},t)$$

Here, $\eta(\mathbf{x}, t)$ is a noise term representing the random flux of particles, identical to the RD process. $\nu\nabla^2 h$ is a diffusion term. The Laplacian $\nabla^2 h$ is a measure of the local surface curvature. Where the surface is peaked (positive curvature), the term is negative,

causing the height to decrease. Where it is in a valley (negative curvature), the term is positive, causing the height to increase. This term therefore systematically drives the surface towards a flatter state. Because it is linear in h, it is known as a linear model. For a 1D substrate, this model predicts a growth exponent of $\beta = 1/4$, indicating a much slower roughening process than RD.

3.3 Kardar–Parisi–Zhang (KPZ) Model

While the EW model accounts for smoothing, it misses another critical aspect of many real growth processes: local, slope-dependent growth. In many systems, particles arriving at the surface are more likely to incorporate at the edges of existing steps or mounds rather than on flat terraces. This creates a "lateral" or "sideways" growth that causes wider features to grow faster. The growth front, therefore, tends to advance perpendicular to the local surface.

The KPZ model extends the EW model by adding a non-linear term to capture this effect:

$$\frac{\partial h(\mathbf{x},t)}{\partial t} = \nu\nabla^2 h(\mathbf{x},t) + \frac{\lambda}{2}(\nabla h(\mathbf{x},t))^2 + \eta(\mathbf{x},t)$$

$\frac{\lambda}{2}(\nabla h)^2$, is proportional to the square of the local surface slope (∇h). It is always positive, meaning it always contributes to increasing the height. Since it is larger where the slope is steeper, it causes mounds to grow faster than valleys, leading to a different kind of roughening than the purely random deposition. This non-linear feedback is a hallmark of many complex systems. For a 1D substrate, the KPZ model predicts a growth exponent of $\beta \approx 1/3$.

3.4 Ballistic Deposition (BD) Model

Ballistic Deposition represents a discrete, atomistic approach that naturally incorporates geometric effects absent from continuum models. In the BD model, particles follow straight-line (ballistic) trajectories toward the substrate. Upon arrival at a site, the particle is deposited on top of the highest point in its immediate neighborhood, including the site itself and its nearest neighbors.

The primary physical phenomenon captured by the BD model is the **ballistic shadowing effect**. This purely geometric mechanism occurs when particles cannot reach valleys that are shadowed by peaks. As peaks receive more flux, they grow faster, amplifying the effect and leading to the formation of porous, columnar microstructures characteristic of low-temperature physical vapor deposition.

Unlike the EW and KPZ models, which rely on thermal diffusion and chemical binding, BD's morphology is determined by flux geometry and surface topology. This makes it particularly suitable for simulating oblique-angle deposition, where the incident flux arrives at grazing angles.

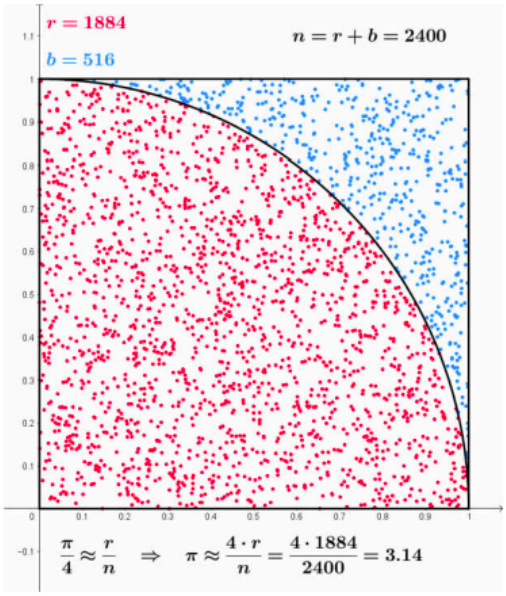

Figure 1: Monte Carlo Method example

4 The Monte Carlo Method

The Monte Carlo (MC) method is a family of computational techniques that use repeated random sampling to find solutions to complex problems. The core idea is to use randomness to solve problems that might be deterministic in principle but are too complex to solve analytically. Instead of solving a set of equations, the underlying process is directly simulated using a random number generator and the outcomes are observed. By running the simulation many times, one can deduce the average behavior of the system.

4.1 Random Number Generation

The simplest models implemented in this project (RD, EW, and KPZ) use direct random number generation for decision-making. Key decisions in the simulation are made by sampling from a uniform random distribution. For example:

- **Atom Deposition:** A column on the substrate is selected by generating a random integer between 0 and $L - 1$, where each integer has an equal probability of being chosen.
- **Diffusion Direction:** In the EW model, the decision to attempt a hop to the left or right is made by randomly choosing between -1 and $+1$.

This direct sampling is computationally efficient and sufficient for modeling the basic rules of RD, EW, and KPZ. However, it is not always physically realistic, as it does not account for the underlying thermodynamics that govern atomic motion.

4.2 The Metropolis Algorithm

A more sophisticated technique is the Metropolis algorithm. It is designed to simulate a system in thermal equilibrium at a finite temperature T. The goal is not just to sample

randomly, but to sample states with a probability that reflects their thermodynamic likelihood, as described by the Boltzmann distribution:

$$P(E) \propto e^{-\frac{E}{k_B T}}$$

where E is the energy of a state, and k_B is the Boltzmann constant. This means low-energy states are more probable than high-energy states.

The Metropolis algorithm works as follows:

1. Start the system in a valid state i with energy E_i.
2. Propose a random change to move to a new state j with energy E_j, here, an atom hopping to a neighboring site.
3. Calculate the change in energy, $\Delta E = E_j - E_i$.
4. **Decision Rule:**
    - If $\Delta E \leq 0$, the move is to a lower (or equal) energy state. This is always favorable. Accept the move.
    - If $\Delta E > 0$, the move is to a higher energy state. This is unfavorable, but not impossible at finite temperature. Accept the move with probability $P = e^{-\frac{\Delta E}{k_B T}}$. This is tested by generating a uniform random number $r \in [0, 1)$. If $r < P$, the move is accepted; otherwise, it is rejected, and the system remains in state i.

By repeating this process many times, the algorithm ensures that the system explores its state space, eventually visiting states with the correct thermodynamic probability. This allows atoms to occasionally move against energy gradient, a crucial process for overcoming energy barriers and achieving large-scale smoothing.

4.3 Kinetic Monte Carlo (KMC)

While the Metropolis algorithm is designed for equilibrium systems, thin film growth is a fundamentally non-equilibrium, dynamic process. Kinetic Monte Carlo addresses this by explicitly modeling the time evolution of the system through physically meaningful transition rates.

The key distinction is that KMC simulates **rare events**—transitions over energy barriers—rather than thermal vibrations. Each possible event i (such as an atom hopping from one site to another) occurs with a rate r_i given by the Arrhenius equation:

$$r_i = \nu_0 \exp\left(-\frac{E_a^i}{k_B T}\right)$$

where ν_0 is the pre-exponential factor (attempt frequency, typically $\sim 10^{12}$ s^{-1}), and E_a^i is the activation energy barrier for that specific event.

KMC fundamentally differs from both direct Monte Carlo (simple random sampling) and Metropolis Monte Carlo (equilibrium sampling). The key idea is that thin film growth involves rare events - transitions over energy barriers separated by long periods

of thermal vibration.
KMC models the system as continuous-time Markov chain where transitions occur stochastically with physically meaningful rates. KMC filters out irrelevant fast vibrations and focuses computational effort on important barrier-crossing events. This provides a speedup of many orders of magnitude.

The standard KMC algorithm, known as the Bortz-Kalos-Lebowitz (BKL) or n-fold way algorithm, proceeds as follows:

1. **Build Event Catalogue:** Identify all possible events that can occur in the current system state, including deposition and diffusion of each mobile adatom.
2. **Calculate Rates:** Compute the rate r_i for each event using the Arrhenius equation.
3. **Calculate Total Rate:** Sum all rates: $R_{tot} = \sum_i r_i$.
4. **Select Event:** Choose which event occurs using probability-weighted selection proportional to event rates.
5. **Execute Event:** Update the system state and return to step 1.

5 Implementation

The project was implemented in Python, leveraging the `numpy` library for efficient numerical array operations and `matplotlib` for visualization. The progression from 1D to 3D implementations and from simple to sophisticated algorithms demonstrates the hierarchical nature of thin film growth modeling.

5.1 1D Implementations

5.1.1 Implementation of Random Deposition (RD)

The Random Deposition model provides the fundamental engine for particle arrival. Its implementation is direct and serves as the foundation for the other models.

- **Initialization:** A 1D array of specified length is created with all elements initialized to zero, representing a perfectly flat substrate.
- **Main Loop:** A loop executes once for each atom being deposited.
- **Deposition Event:** A column index is selected randomly, and the height at that index is incremented by one.
- **Core Principle:** This isolates the effect of purely random particle flux with no other physical interactions.

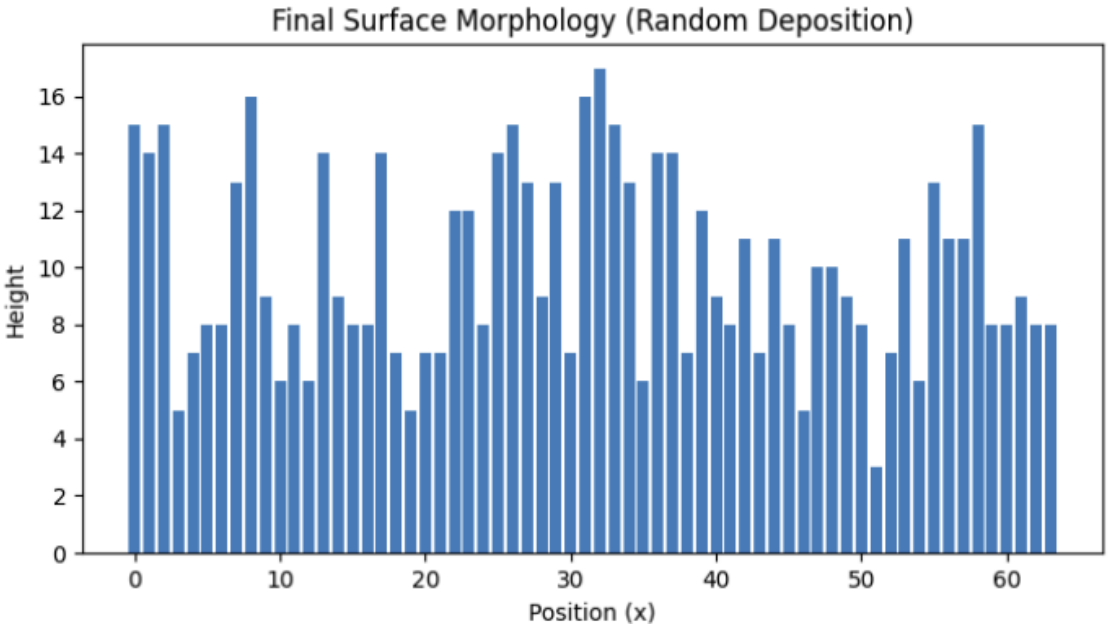

Figure 2: Random Distribution Surface Topology

5.1.2 Implementation of Edwards-Wilkinson (EW)

The EW model introduces surface relaxation by adding a diffusion mechanism after each deposition event.

- **Deposition:** Random column selection and height increment, identical to RD.
- **Post-Deposition Diffusion:** A secondary loop runs for a predefined number of diffusion attempts. In each attempt, a random direction (left or right) is chosen, and if the neighboring site has lower height, the atom hops to that neighbor.
- **Core Principle:** This "downhill only" movement is a zero-temperature approximation of surface-tension-driven smoothing.

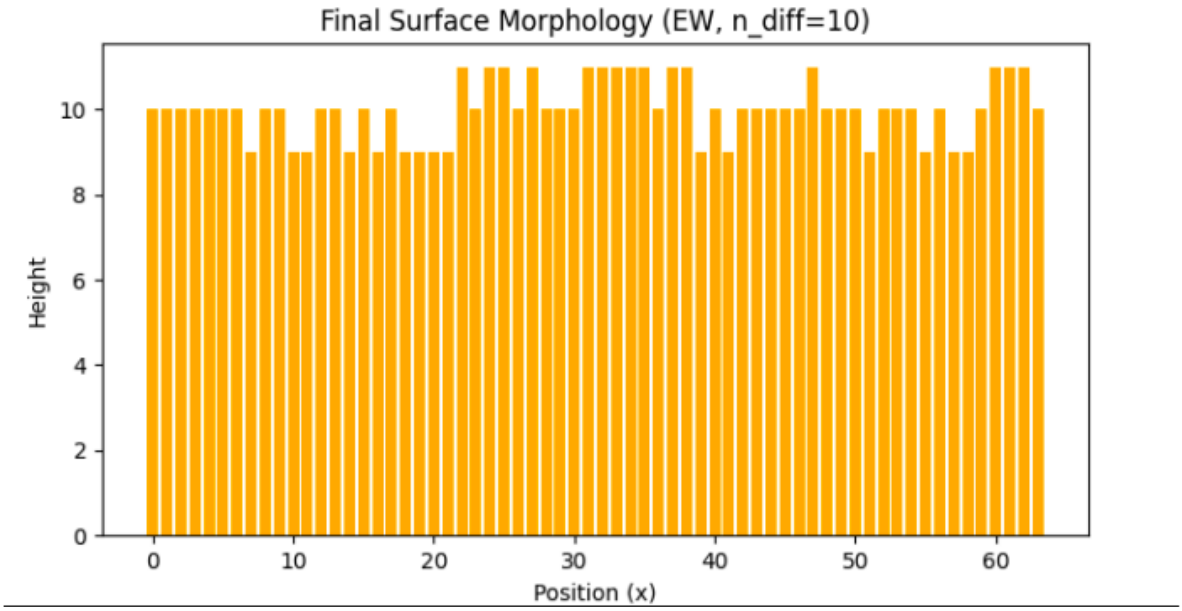

Figure 3: EW model Surface Topology

5.1.3 Implementation of Kardar-Parisi-Zhang (KPZ)

The KPZ model modifies the deposition process to account for lateral, slope-dependent growth.

- **Site Selection:** A random column is selected for particle landing.
- **Pre-Deposition Check:** With a certain probability, a lateral growth mechanism is triggered.
- **Lateral Growth Rule:** If triggered, the target column's height is raised to match the height of its taller neighbors before final deposition.
- **Final Deposition:** The column height is incremented by one.
- **Core Principle:** This probabilistic rule models the non-linear KPZ term, promoting growth perpendicular to the local surface slope.

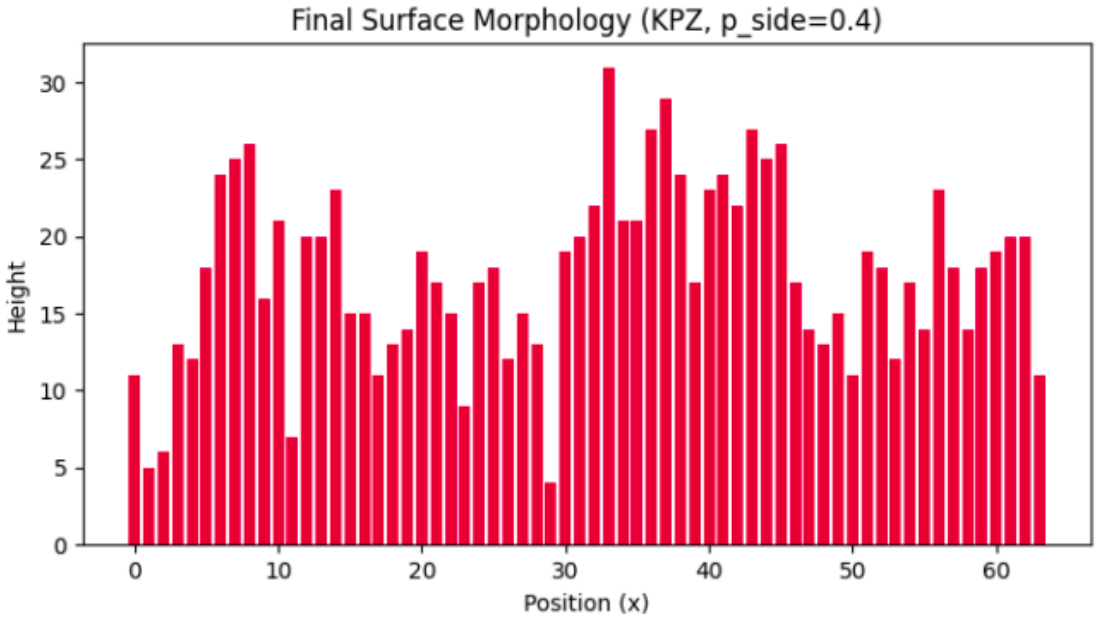

Figure 4: KPZ model Surface Topology

5.2 2D implementation with Metropolis Relaxation

The natural extension of the 1D to 2D substrates provides more realistic representations of actual thin film growth, where surface topology plays a critical role.

5.2.1 2D Edwards-Wilkinson Implementation

The 3D EW model extends the linear relaxation mechanism to a 2D substrate (with height as the third dimension):

- The substrate is represented as a 2D array `h[x, y]` where each element stores the column height.
- Deposition occurs at a randomly selected (x, y) position.
- Diffusion attempts consider all four nearest neighbors in the 2D plane.
- Periodic boundary conditions are applied in both x and y directions.
- The roughness calculation accounts for the 2D nature: $w = \sqrt{\langle (h - \bar{h})^2 \rangle}$ where the average is over all $L \times L$ sites.

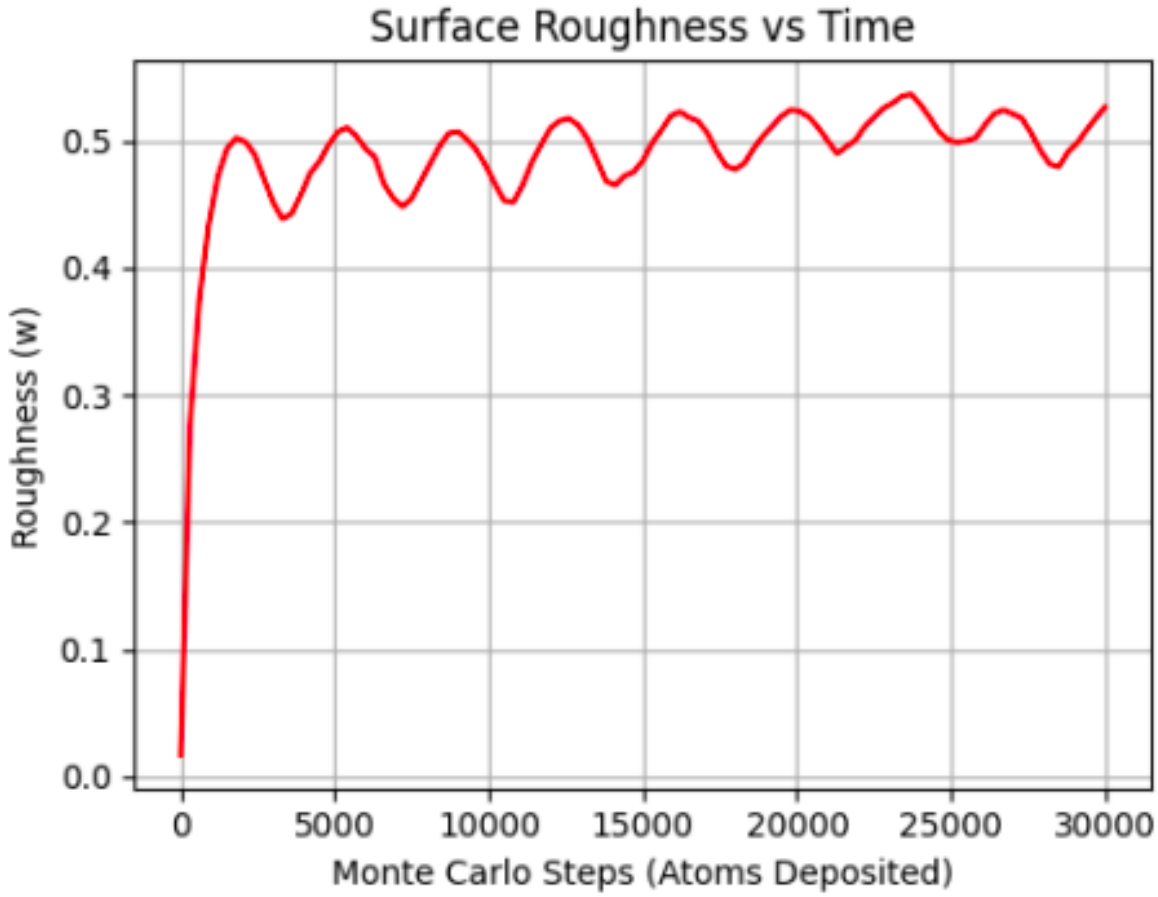

Figure 5: 2D EW model Surface Topology

5.2.2 2D Kardar-Parisi-Zhang Implementation

The 3D KPZ model similarly extends lateral growth to 2D substrates:

- Lateral growth checks all four neighbors in the 2D plane.
- The height-matching rule applies to the maximum height among all four neighbors.
- This creates more complex mound structures than in 1D, as growth can propagate in multiple directions.

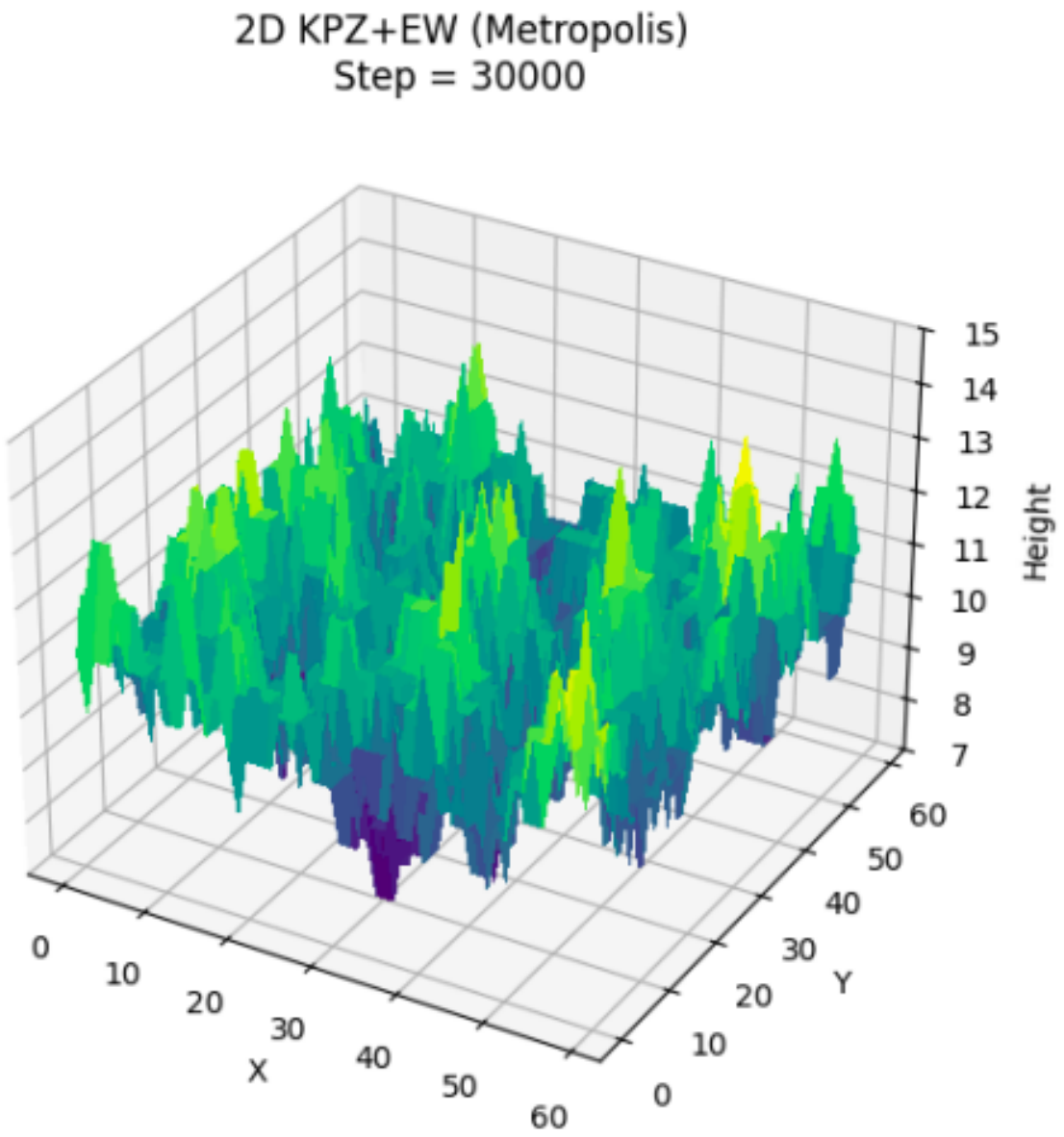

Figure 6: 2d KPZ model Surface Topology

5.2.3 Ballistic Deposition

The 2D Ballistic Deposition model extends the growth simulation to a realistic two-dimensional substrate while incorporating thermally-activated relaxation through the Metropolis algorithm.

- Model Description The simulation operates on a 2D lattice with periodic boundary conditions. Each Monte Carlo step consists of two phases:

    1. **Ballistic Deposition Phase (Roughening):** A random site (x, y) is selected. The particle is deposited on top of the highest point among the site itself and its four nearest neighbors (left, right, up, down).

2. **Metropolis Diffusion Phase (Smoothing):** Following deposition, multiple diffusion attempts are made. For each attempt:
   - A random site with at least one atom is selected.
   - A random neighbor is chosen for a potential hop.
   - The energy change ΔE for the proposed hop is computed.
   - The hop is accepted according to the Metropolis criterion: always if $\Delta E \leq 0$, otherwise with probability $\exp(-\Delta E/kT)$.

This hybrid approach combines the geometric effects of ballistic aggregation with thermally-activated surface relaxation, providing a more realistic model than either mechanism alone.

- Physical Parameters Key parameters controlling the model's behavior include:
  - **Temperature (kT):** Controls the acceptance probability for energetically unfavorable hops. Higher temperatures allow more uphill diffusion and greater surface smoothing.
  - **Surface Tension (J):** Determines the strength of the smoothing force. Higher values increase the energy penalty for rough surfaces.
  - **Diffusion attempts per deposition:** Controls the relative timescales of roughening and smoothing processes.

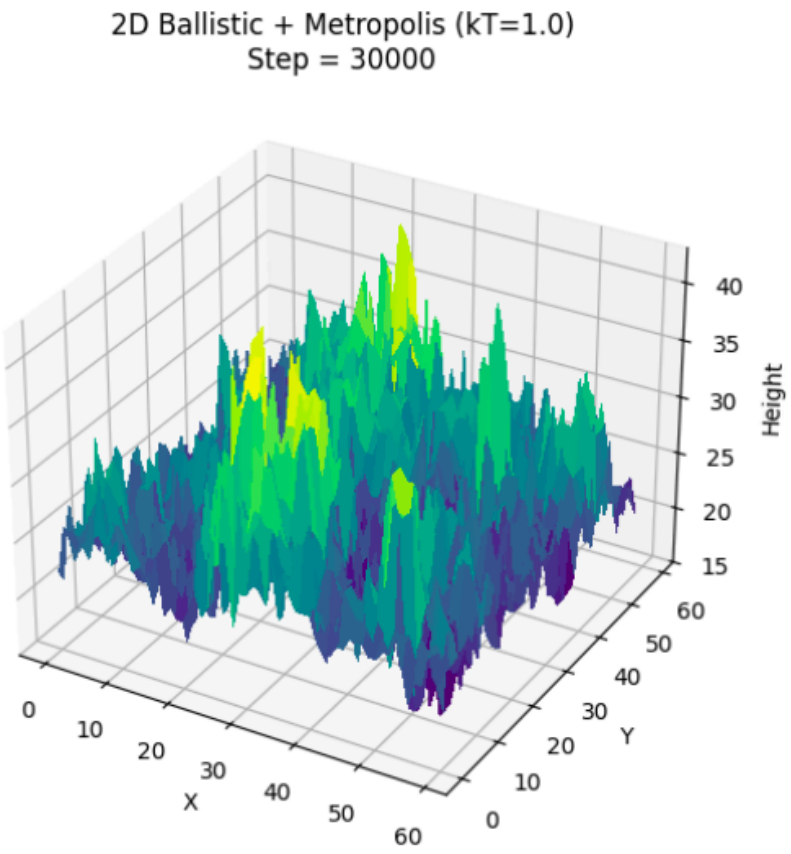

Figure 7: 2D Ballistic model Surface Topology

5.3 Material-Specific Kinetic Monte Carlo Implementation

The most advanced implementation in this project is a fully material-specific KMC simulation that incorporates realistic physical parameters and temperature-dependent kinetics.

5.3.1 Physical Framework

The simulation models a 2D lattice representing a crystalline substrate where each site can be occupied by atoms. The key physical processes included are:

1. **Deposition:** Atoms arrive at the surface with a flux F (atoms per site per second). The total deposition rate is $R_{dep} = F \times L^2$, where L is the lattice size.

2. **Surface Diffusion:** Adatoms can hop to neighboring sites if they are not embedded (i.e., if at least one neighbor is lower). The diffusion rate depends on the activation energy. The diffusion rate is:

$$r_{\text{diff}} = \nu_0 \exp\left(-\frac{E_a}{k_B T}\right)$$

5.3.2 Material-Specific Parameters

The realism of the simulation is achieved through material-specific input parameters:

- **Temperature (T):** Substrate temperature in Kelvin, the primary control parameter for diffusion kinetics.
- **Deposition Flux (F):** Controls the arrival rate of atoms (atoms per site per second).
- **Pre-exponential Factor (ν_0):** Attempt frequency, typically 10^{12} s^{-1} for atomic vibrations.
- **Base Diffusion Energy (E_a^{base}):** Activation barrier for an isolated adatom to hop on the surface (in eV).
- **Lateral Binding Energy (E_a^{lateral}):** Additional energy barrier per lateral neighbor (in eV).

Different materials are simulated by using material-specific values for these parameters, which can be obtained from experimental measurements. For example:

- High E_a^{base} materials exhibit limited surface diffusion, leading to rougher, more columnar growth.
- Low E_a^{base} materials show extensive diffusion, producing smoother, more compact films.

5.3.3 Algorithm Implementation

The BKL algorithm is implemented as follows:

1. **Event Construction:** For each simulation step, all possible events are enumerated:
    - One deposition event (can occur at any of the L^2 sites).
    - Diffusion events for each non-embedded surface atom (4 possible directions each).
2. **Rate Calculation:** Each event's rate is calculated using the Arrhenius equation. For diffusion, the activation energy depends on the local atomic environment (number of lateral neighbors).
3. **Event Selection:** A cumulative probability distribution is constructed from the rates, and an event is selected via inverse transform sampling.
4. **State Update:** The selected event is executed (atom deposited or moved), and the system state is updated.

5.3.4 Output and Analysis

The simulation tracks several key metrics over time:

- **RMS Roughness:** Quantifies surface morphology evolution.
- **Mean Height:** Tracks total film thickness.

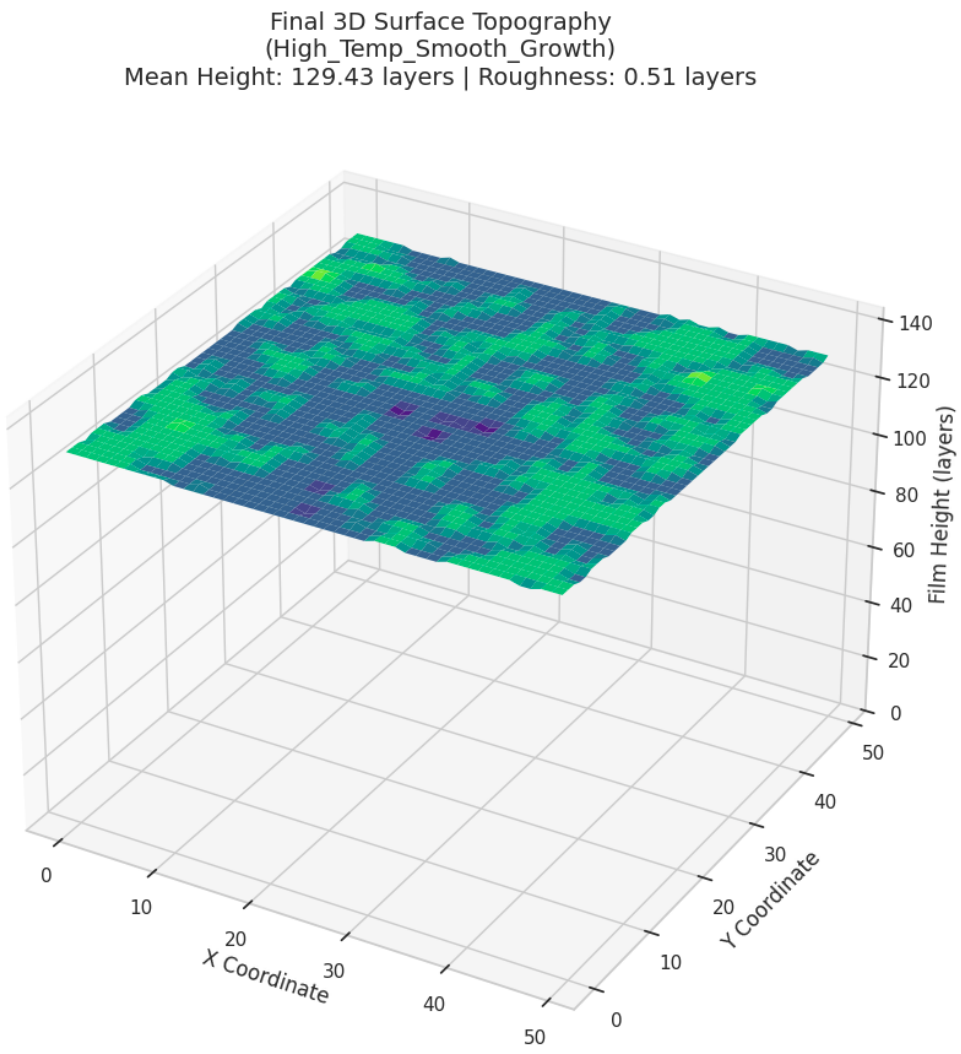

Figure 8: 2D KMC model Surface Topology

This material-specific KMC framework represents the state-of-the-art in computationally efficient, yet physically realistic, thin film growth simulation. By varying the input parameters, one can simulate different materials, different substrates, and different growth conditions, making it a powerful predictive tool for materials design.

6 Results and Discussion

6.1 Comparison of 1D Growth Models

The one-dimensional implementations of RD, EW, and KPZ models demonstrate the progressive incorporation of physical mechanisms and their effects on surface roughening. Analysis of roughness evolution over time reveals:

- **Random Deposition:** Exhibits the fastest roughening with growth exponent $\beta \approx 0.5$, consistent with Poissonian statistics.
- **Edwards-Wilkinson:** Shows reduced roughening ($\beta \approx 0.25$) due to the smoothing effect of surface diffusion. The linear relaxation mechanism effectively suppresses small-scale fluctuations.
- **Kardar-Parisi-Zhang:** Displays intermediate roughening ($\beta \approx 0.33$) reflecting the competition between the smoothing term and the roughening non-linear term.

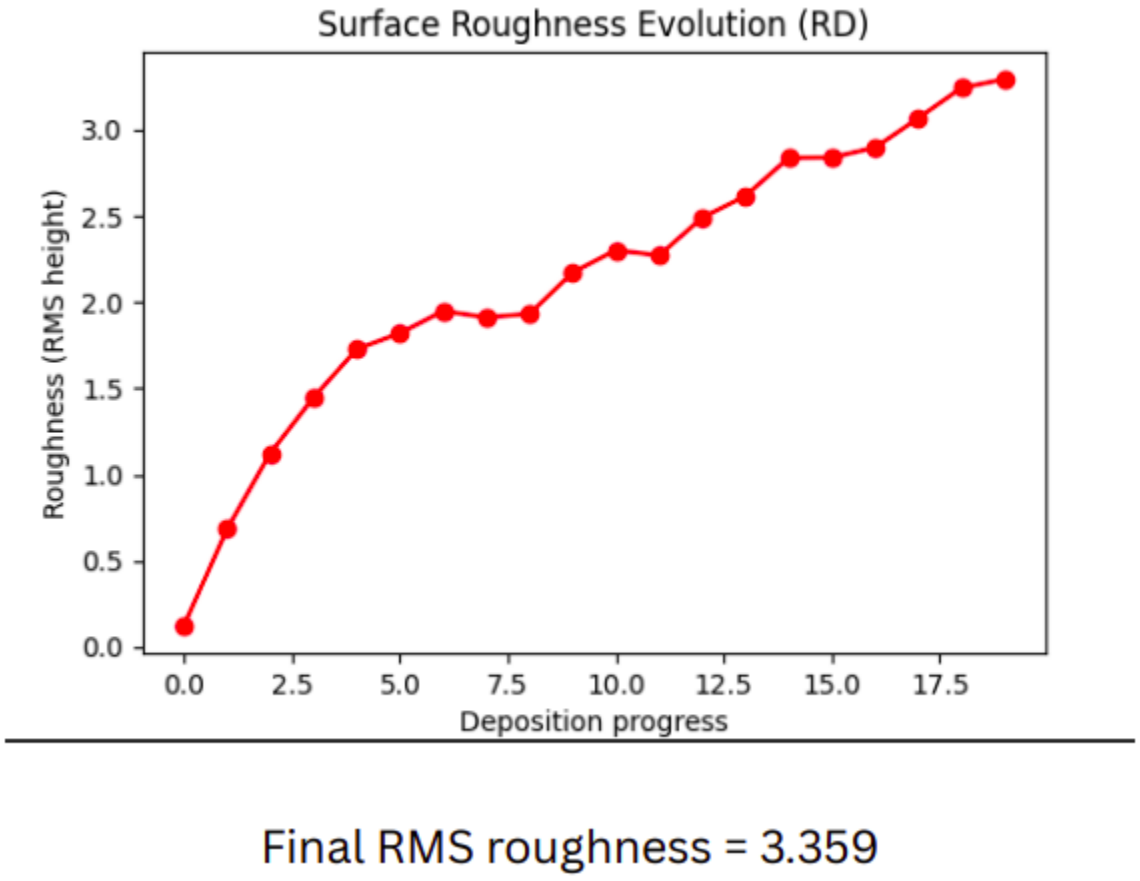

Figure 9: Surface Roughenss growth of 1D Random Distribution model

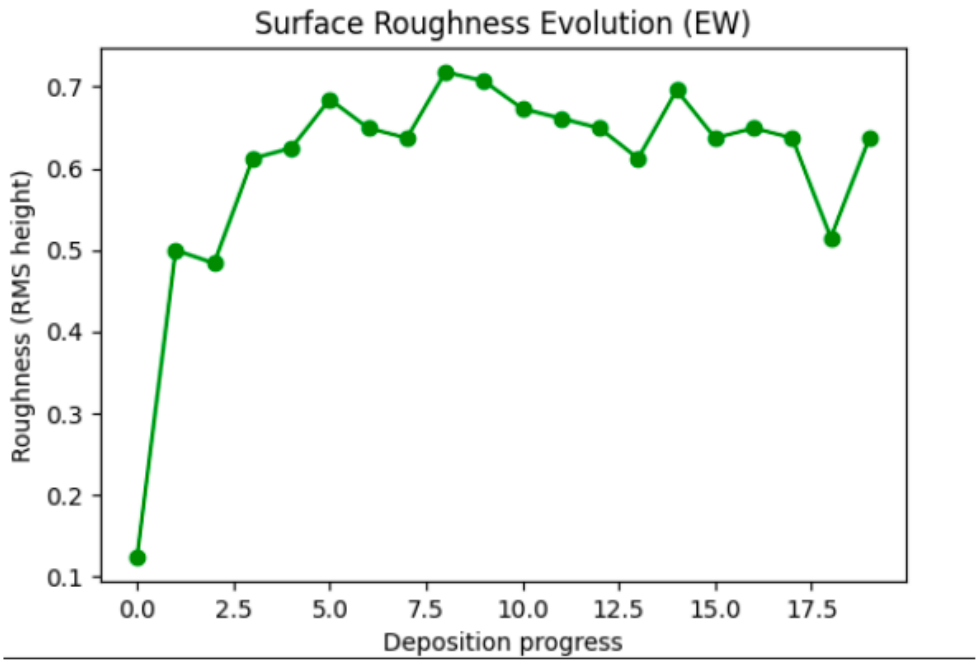

Figure 10: Surface Roughenss growth of 1D EW model

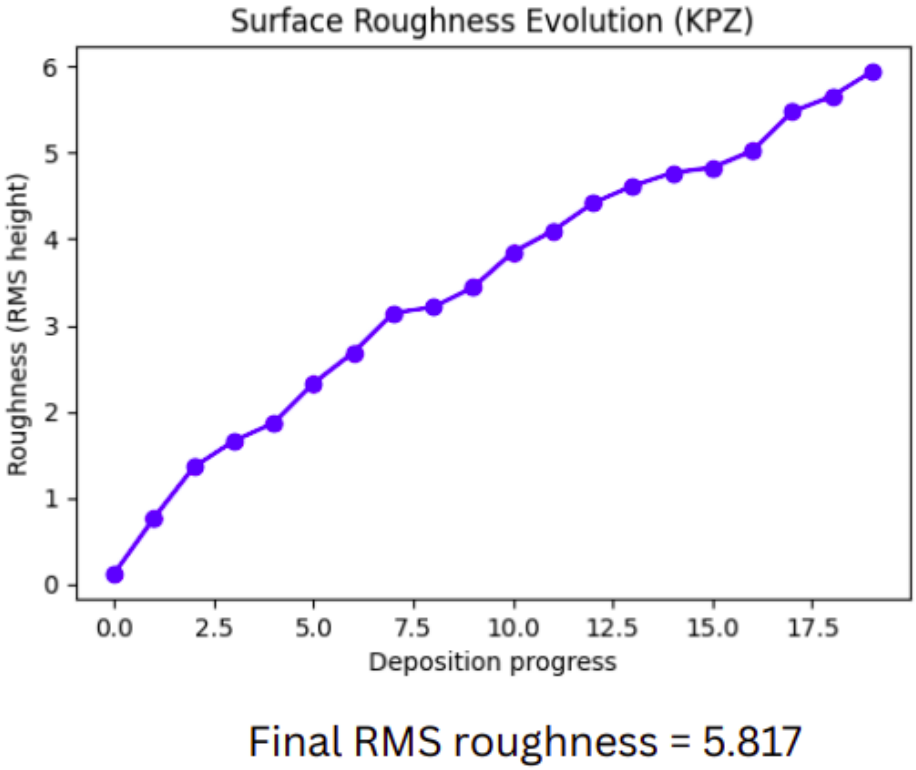

Figure 11: Surface Roughenss growth of 1D KPZ model

These results validate the simulation implementations, as the extracted exponents

match theoretical predictions.

6.2 Dimensional Effects: 1D vs 2D

Extension to two-dimensional substrates reveals important dimensional dependencies. The 2D surface (with height as the third dimension) exhibits qualitatively different behavior:

- The EW model in 2D shows much slower roughening, with near-logarithmic growth. This reflects the increased effectiveness of surface relaxation when atoms have four neighboring sites rather than two.
- The KPZ model in 2D develops more complex mound structures. The non-linear term in 2D creates asymmetric features that cannot occur in 1D.

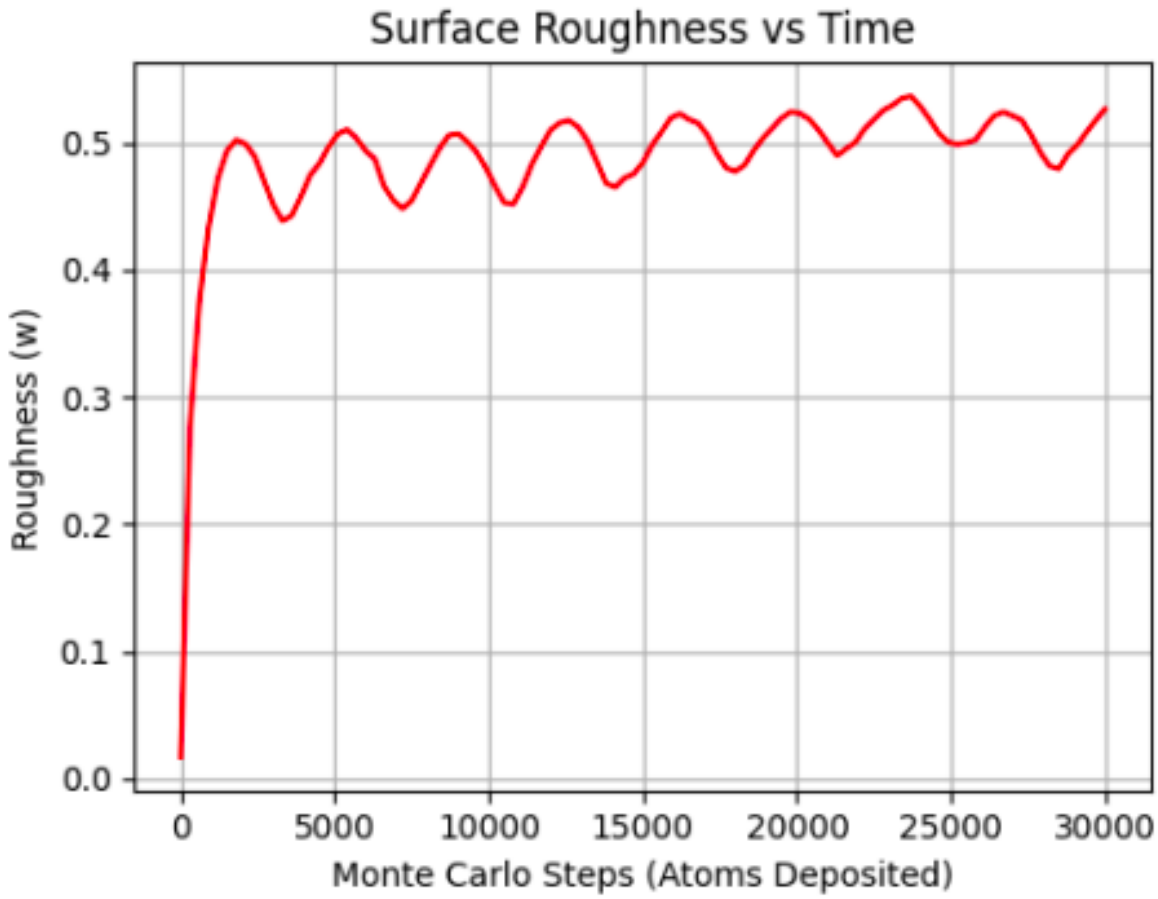

Figure 12: Surface Roughenss growth of 2D EW model

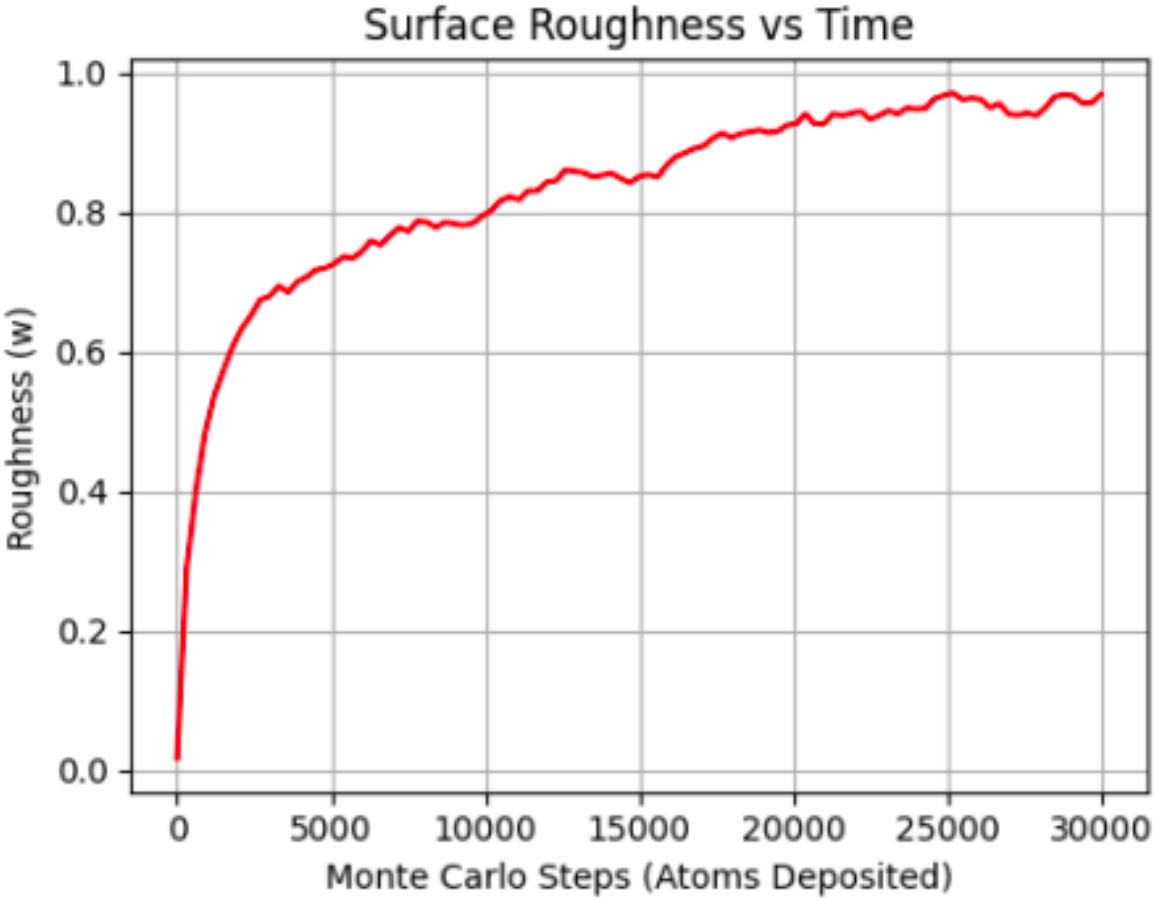

Figure 13: Surface Roughenss growth of 2D KPZ model

6.3 Ballistic Deposition with Metropolis Relaxation

The Ballistic Metropolis model demonstrates the interplay between roughening and smoothing mechanisms:

- At low effective temperature ($kT \ll J$), the Metropolis acceptance probability approaches zero for uphill moves. Growth resembles pure ballistic deposition with high roughness and columnar features.
- At high effective temperature ($kT \gg J$), uphill moves are frequently accepted. Surface diffusion becomes efficient, smoothing the ballistic roughness and producing denser films.
- At intermediate temperatures, competition between ballistic aggregation and thermal relaxation produces microstructures characteristic of real physical vapor deposition.

Varying the temperature parameter directly demonstrates how experimental control of substrate temperature influences film morphology, providing a bridge between simulation and real deposition processes.

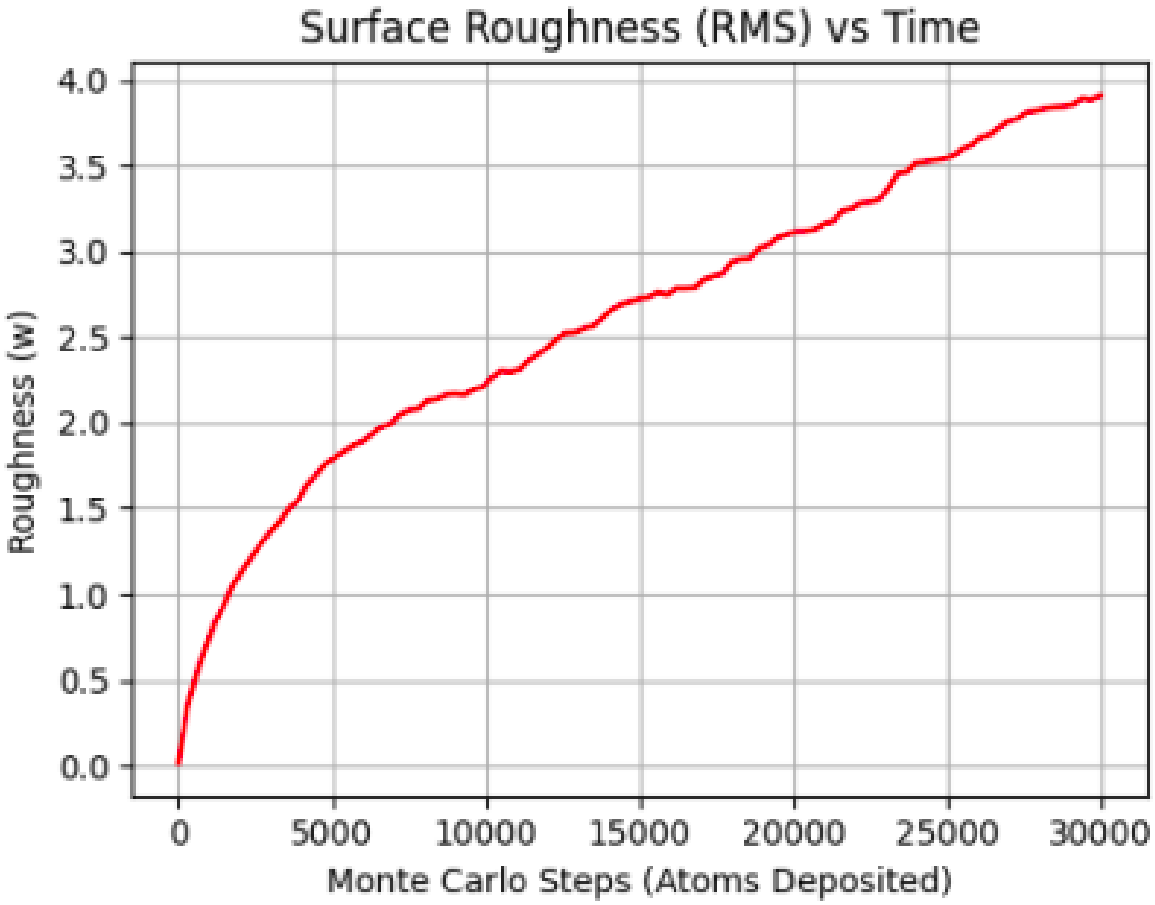

Figure 14: Surface Roughenss growth of 2D Ballistic model

6.4 Material-Specific KMC: Temperature and Flux Effects

The full KMC implementation reveals the rich phase space of thin film growth:

6.4.1 Temperature Dependence

Simulations at different temperatures with fixed flux show distinct morphological regimes:

- **Low Temperature ($T < 400$ K):** Limited diffusion leads to kinetically-limited growth. Atoms stick near where they land, producing rough surfaces with columnar features. The growth exponent approaches that of ballistic deposition.
- **Intermediate Temperature ($400 < T < 800$ K):** Diffusion becomes significant but not dominant. Island nucleation and growth occur, with characteristic island densities and sizes. Surface roughness is moderate.
- **High Temperature ($T > 800$ K):** Extensive diffusion leads to thermodynamically-limited growth. Atoms find low-energy sites before being covered by new arrivals. Smooth, compact films with faceted features emerge. The growth exponent approaches that of EW-like behavior.

6.4.2 Flux Dependence

At fixed temperature, varying the deposition flux reveals:

- **Low Flux:** Adatoms have time to diffuse extensively before the next atom arrives. Island density is low, and growth is smooth.
- **High Flux:** Many atoms arrive before diffusion can occur. Island density is high, and surfaces are rougher due to limited relaxation.

6.4.3 Material Comparison

By varying the activation energy parameters, the simulation demonstrates material-specific growth:

- Materials with low E_a^{base} (e.g., noble metals on close-packed surfaces) exhibit high mobility and smooth growth.
- Materials with high E_a^{base} (e.g., covalently bonded systems) show limited diffusion and rough, porous morphologies.
- Materials with strong lateral binding (E_a^{lateral}) form stable islands earlier, affecting nucleation density.

This demonstrates the framework's capability to simulate different materials by simply changing input parameters, achieving the project's core objective.

7 Conclusions

This project has developed a framework for simulating thin film deposition and growth using Monte Carlo methods. The progression from simple one-dimensional models to three-dimensional, material-specific simulations demonstrates the complexity of modelling nanoscale scenarios.

7.1 Achievements

1. **Implementation of Canonical Models:** Successfully implemented RD, EW, and KPZ models in both 1D and 3D, with extracted growth exponents consistent with theoretical predictions.
2. **Ballistic Deposition with Thermal Relaxation:** Developed a hybrid 2D model combining geometric shadowing effects with Metropolis-based thermal relaxation, capturing the interplay between roughening and smoothing mechanisms.
3. **Material-Specific Kinetic Monte Carlo:** Implemented a full KMC simulation with temperature-dependent diffusion kinetics, material-specific activation energies, and proper rare-event dynamics.

7.2 Limitations

While the current implementation successfully captures many characteristics of nanofilm growth, several limitations present scope for future improvements:

- The KMC model uses a rigid square lattice, which cannot represent amorphous growth.
- Desorption is not yet implemented but would extend applicability to chemical vapor deposition and reactive processes.
- Experimental validation through direct comparison experimental would provide quantitative assessment of predictive accuracy.

The framework developed in this project established a versatile platform for computational materials design in thin film systems.

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