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ATOMISTIC MOLECULAR DYNAMICS SIMULATION OF CU THIN-FILM GROWTH UNDER MOLECULAR BEAM EPITAXY CONDITIONS: EFFECTS OF SUBSTRATE TEMPERATURE AND INCIDENT KINETIC ENERGY

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ABSTRACT

A molecular dynamics framework was developed to examine the combined influence of substrate temperature and incident kinetic energy on Cu-on-Cu(001) thin-film growth under molecular beam epitaxy (MBE) conditions. The simulations solve Newton's equations of motion using the Mishin embedded-atom method (EAM) potential for Cu-Cu interactions, while incident Cu atoms are introduced normal to the surface with kinetic energies of 0.1, 1, and 5 eV. Substrate temperatures of 300, 500, and 700 K generate a 3 x 3 process matrix. The deposited layer is quantified using vertical extent, RMS vertical spread, coordination number, and average atomic potential energy. The results reveal a non-monotonic morphology response: at 500 and 700 K the 1 eV condition gives the smallest RMS vertical spread, whereas 5 eV increases local coordination and produces a more negative deposited-atom potential energy but also a larger vertical dispersion. The study therefore identifies a competition between impact-assisted atomic rearrangement and morphology roughening. Because the atom arrival rate accessible to MD is much higher than experimental MBE fluxes, the model is interpreted in terms of relative atomistic trends rather than direct experimental growth rates.

Keywords: Molecular Dynamics; Molecular Beam Epitaxy (MBE); Cu(001); Copper Thin Film; Incident Energy; Substrate Temperature; Embedded-Atom Method; Surface Morphology; Coordination Number

1 INTRODUCTION

Controlled deposition of metallic thin films is central to semiconductor interconnects, seed layers, diffusion-barrier architectures, microelectromechanical systems, and a wide range of functional coatings. Copper is especially important because of its high electrical and thermal conductivity and its extensive use in metallization. At the same time, the local structure of a deposited Cu film, its surface roughness, defect population, and interface mixing depend strongly on the energetic and thermal conditions under which incoming atoms arrive at the growth surface. Molecular beam epitaxy and related physical-vapor-deposition methods exploit the relationship among incoming flux, substrate temperature,

surface diffusion, nucleation, and step incorporation to control film morphology [1,2]. Even for a chemically simple homoepitaxial system such as Cu on Cu, the atomistic pathways that connect an incident atom to an adsorbed, exchanged, or incorporated configuration are highly dynamic and cannot be completely inferred from a static final micrograph.

The classic description of thin-film growth distinguishes layer-by-layer, island, and mixed growth modes according to the balance between film-film and film-substrate interactions and the kinetics of surface transport [2]. For an incoming metal atom, the available kinetic energy is dissipated through collisions with substrate atoms and through phonon excitation. When that energy is very low, an adatom may become trapped near its first adsorption site, which can favor incomplete layer filling and kinetic roughening. As the incident energy increases, additional surface diffusion, exchange processes, and access to lower-energy adsorption sites become possible. However, excessive kinetic energy can also drive penetration, atomic exchange, local disorder, and defect generation. Temperature has an analogous but not identical influence: thermal activation increases the probability of diffusion and structural rearrangement, but it can also increase configurational fluctuations and promote intermixing when combined with energetic impacts.

Molecular dynamics (MD) is well suited for resolving these short-time atomistic processes because Newton's equations of motion are integrated for every atom while the interatomic potential supplies the force field. For metallic systems, the embedded-atom method (EAM) represents the many-body nature of metallic bonding more realistically than a simple pair potential [3]. The Cu EAM formulation developed by Mishin et al. was specifically assessed against equilibrium and nonequilibrium structures and is widely used for Cu defects, surfaces, deformation, and deposition-related simulations [4]. LAMMPS provides an efficient implementation of MD algorithms and deposition operations [5], while OVITO enables trajectory visualization and local structure analysis [6].

Prior MD studies have shown that incident energy and temperature can alter film growth modes, roughness, intermixing, and defect formation. Jing et al. studied Cu deposition on Cu(001) and reported approximately layer-island growth in the 1-5 eV range with increasing intermixing at higher energy [7]. Hwang et al. found that incident energy was a dominant factor governing deposition mode and roughness during Cu cluster deposition on Si [8]. Gilmore examined energetic Cu deposition on Cu(001) at 5-80 eV and demonstrated exchange, penetration, interstitial formation, and sputtering as the impact energy increased [9]. More recent work on Cu seed-layer deposition on Ta similarly emphasized the coupled effects of incident energy and substrate temperature on surface roughness, interface mixing, and defects [10]. These studies establish that the energy-temperature parameter space is intrinsically competitive: an increase in mobility can improve local packing while simultaneously increasing penetration or roughness under some conditions.

The present work focuses on a deliberately compact Cu-on-Cu(001) model designed to isolate this competition. Instead of attempting to reproduce the experimental deposition rate of an MBE system, the simulations examine relative atomistic trends within a consistent computational protocol. Nine cases are generated from three substrate temperatures, 300, 500, and 700 K, and three normal-incidence energies, 0.1, 1, and 5 eV. For each case, 300 Cu atoms are deposited onto the same Cu(001) substrate. The final deposited group is characterized using four direct metrics: vertical extent, RMS vertical spread, average coordination number, and average potential energy per deposited atom. The time-resolved trajectories are additionally inspected to distinguish initial adsorption from the final film morphology.

The main objective is therefore not to claim an experimentally calibrated MBE growth rate, but to determine whether a low-complexity MD model can reveal systematic process-property relationships that are useful for interpreting Cu thin-film growth. Particular attention is given to three questions. First, does a moderate incident energy reduce or increase the final vertical roughness of the deposited layer? Second, how does temperature modify the local coordination of deposited atoms at fixed incident energy? Third, can the most energetically relaxed deposited configuration also be the roughest configuration? The answers to these questions provide a physically useful basis for expanding the model toward thicker films, longer time scales, structural classification, and process optimization.

2 COMPUTATIONAL METHODOLOGY

2.1 Molecular dynamics model

All simulations were performed using LAMMPS, version 29 August 2024 Update 2, with the metal unit system. The simulated substrate was face-centered-cubic Cu oriented with the (001) free surface normal to the z direction. A lattice parameter of 3.615 Å was used, consistent with the Cu EAM potential file. The in-plane dimensions were 12 × 12 conventional FCC unit cells, while the substrate thickness was six conventional unit cells. The corrected substrate construction contained 3456 atoms. Periodic boundary conditions were imposed along x and y to represent an extended

surface, and a nonperiodic boundary with a large vacuum region was used along z . This geometry avoids interaction between the free surface and an artificial periodic image in the deposition direction.

The bottom part of the substrate was divided into a stationary region and a thermostatted region. The lowest atomic layer was fixed by setting its force and velocity to zero, thereby providing a mechanically stable base. A region above the fixed layer was coupled to a Langevin thermostat at the prescribed substrate temperature. The remaining surface atoms evolved according to an NVE time integrator. This partitioning allows impact energy to be transferred from the deposition zone into the substrate and dissipated through the thermal bath while preventing rigid-body translation of the slab. The global temperature reported by LAMMPS includes atoms outside the thermostat definition; therefore, the imposed bath temperature, rather than the whole-system instantaneous temperature, is the physically relevant substrate-temperature control variable in the present comparison.

Cu-Cu interactions were represented using the Mishin EAM/alloy potential [4]. In EAM, the total energy contains an embedding contribution that depends on the local host electron density together with a pairwise contribution. In a commonly used notation,

$$E_{\text{tot}} = \sum_i F(\rho_i) + \frac{1}{2} \sum_i \sum_{j \neq i} \phi(r_{ij}) \quad (1)$$

where $F(\rho_i)$ is the embedding energy of atom i in the local host electron density, $\phi(r_{ij})$ is the pair interaction, and r_{ij} is the interatomic separation. The local electron density is

$$\rho_i = \sum_{j \neq i} f(r_{ij}) \quad (2)$$

where $f(r_{ij})$ is the electron-density contribution from neighboring atom j . This many-body formulation is appropriate for metallic Cu and is the same class of description used in the Cu-on-Cu(001) MD study of Jing et al. [7].

2.2 Governing equations for the MD-MBE model

The atomistic MBE model is governed by classical mechanics. For each atom i , LAMMPS integrates Newton's equation of motion using forces obtained from the gradient of the many-body potential energy:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i = -\nabla_i U \quad (3)$$

The trajectories are advanced with a Verlet-family time integrator. In compact form, the position and velocity updates can be written as

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t) \Delta t + \frac{\mathbf{F}_i(t)}{2m_i} \Delta t^2 \quad (4a)$$

$$\mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t) + \frac{\mathbf{F}_i(t) + \mathbf{F}_i(t + \Delta t)}{2m_i} \Delta t \quad (4b)$$

where $\Delta t = 1$ fs in the present simulations. This integration scheme is appropriate for resolving the fast collision, adsorption, and surface-relaxation events that occur after each Cu atom arrives at the surface.

The incident kinetic energy defines the normal beam velocity of each Cu atom. For normal incidence,

$$E_{\text{inc}} = \frac{1}{2} m_{\text{Cu}} v_z^2, \quad v_z = \sqrt{\frac{2E_{\text{inc}}}{m_{\text{Cu}}}} \quad (5)$$

Using the Cu atomic mass gives 5.511, 17.426, and 38.966 Å/ps for 0.1, 1, and 5 eV, respectively. Thus the beam energy enters the simulation through the translational kinetic energy rather than by an empirical fitting parameter.

The instantaneous kinetic temperature of a mobile atom group follows from equipartition:

$$T = \frac{2K}{N_f k_B}, \quad K = \sum_i \frac{1}{2} m_i |\mathbf{v}_i - \mathbf{v}_{\text{cm}}|^2 \quad (6)$$

where K is the kinetic energy after removal of center-of-mass motion, N_f is the number of active degrees of freedom, and k_B is the Boltzmann constant. Because the lowest substrate layer is fixed, the physically relevant substrate temperature should be evaluated from the mobile or thermostatted substrate atoms rather than from all atoms.

Thermal control of the substrate is implemented with a Langevin thermostat. Its stochastic equation of motion is

$$m_i \frac{dv_i}{dt} = \mathbf{F}_i - m_i \gamma \mathbf{v}_i + \mathbf{R}_i(t) \quad (7)$$

where γ is the damping coefficient and $\mathbf{R}_i(t)$ is a random force satisfying the fluctuation-dissipation relation. This term removes the excess impact energy deposited by incoming atoms and mimics heat transfer from the finite MD slab to a larger thermal reservoir.

For MBE interpretation, the atom arrival rate is conveniently expressed as an areal deposition flux:

$$J = \frac{N_{\text{dep}}}{A t_{\text{dep}}} \quad (8)$$

For the present $12a \times 12a$ surface ($a = 3.615 \text{ \AA}$), $\text{\AA} = 1.881 \times 10^{-17} \text{ m}^2$. Depositing 300 atoms in 30 ps corresponds to J approximately $5.32 \times 10^{29} \text{ atoms m}^{-2} \text{ s}^{-1}$. This value is intentionally far above experimental MBE fluxes because conventional MD accesses picosecond-to-nanosecond timescales. Consequently, the simulation should be used to compare relative temperature and incident-energy effects rather than to reproduce an experimental growth rate.

A useful retention descriptor is the sticking coefficient

$$S = \frac{N_{\text{retained}}}{N_{\text{incident}}} \quad (9)$$

where N_{retained} is the number of deposited atoms remaining in the simulation after relaxation. All nine present cases retain the 300 inserted atoms, giving $S = 1$ within the simulated time window and low-energy range.

where F_i is the embedding energy of atom i in the local electron density ρ_i , ϕ_{ij} is the pair interaction between atoms i and j , and r_{ij} is their separation. This many-body form is important for metallic surfaces because the coordination environment of a surface or deposited atom differs strongly from that of a bulk atom [3,4].

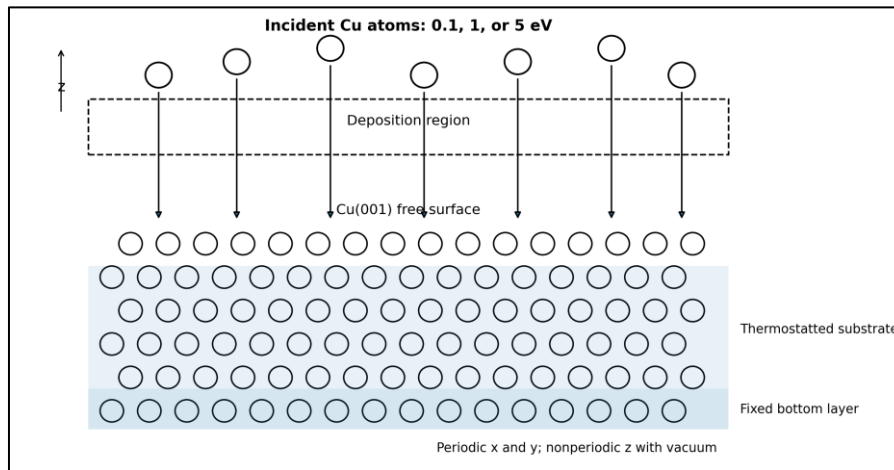


Figure 1: Schematic of the Cu-on-Cu(001) deposition model used in the simulations. Incoming Cu atoms were introduced above the free surface with a prescribed normal velocity. The lower substrate contained a fixed layer and a thermostatted region, with periodic boundary conditions in x and y and vacuum along z.

2.3 Deposition protocol and parameter matrix

A timestep of 0.001 ps, equivalent to 1 fs, was used throughout. Each substrate was first energy-minimized and then equilibrated for 10,000 steps. Deposition was subsequently performed for 30,000 steps, followed by 20,000 steps of post-deposition relaxation. The same simulation schedule was repeated for every temperature-energy combination. Three substrate temperatures were selected: 300, 500, and 700 K. Three incident energies were selected: 0.1, 1, and 5 eV. This produced nine simulations in total.

For a Cu atom of mass m , the prescribed normal impact velocity was calculated from the classical kinetic-energy relationship $E = (1/2)mv^2$. Using Cu mass in the LAMMPS metal unit system, the implemented conversion was which gives incident speeds of 5.511, 17.426, and 38.966 $\text{\AA}/\text{ps}$ for 0.1, 1, and 5 eV, respectively. A total of 300 Cu atoms was inserted in each case, one atom every 100 timesteps. Because 100 timesteps correspond to 0.1 ps, the computational

deposition rate was 10 atoms/ps. This rate is intentionally much higher than an experimental MBE flux because classical MD can access only nanosecond and sub-nanosecond time scales. Consequently, all conclusions are interpreted as relative atomistic trends across a controlled parameter matrix rather than direct predictions of laboratory growth rate.

Table 1: Molecular dynamics deposition parameters.

Parameter	Value
Substrate	FCC Cu(001)
Initial substrate atoms	3456
Lattice parameter	3.615 Å
In-plane cell size	12 x 12 conventional FCC cells
Substrate thickness	6 conventional FCC cells
Boundary conditions	Periodic x, y; nonperiodic z with vacuum
Interatomic potential	Mishin Cu EAM/alloy
Timestep	1 fs
Substrate temperatures	300, 500, 700 K
Incident energies	0.1, 1, 5 eV
Deposited Cu atoms per case	300
Equilibration	10 ps
Deposition	30 ps
Post-deposition relaxation	20 ps
Total simulated time per case	60 ps

2.4 Film metrics and trajectory analysis

The deposited atoms were stored as a separate LAMMPS group, allowing film-specific statistics to be calculated after the relaxation stage. Four principal metrics were extracted. The vertical extent was defined as $z_{\max} - z_{\min}$ for the deposited group. This metric is sensitive to isolated high or low atoms and therefore acts as a peak-to-peak measure of the deposited configuration rather than a conventional engineering surface-roughness parameter.

The deposited-layer vertical extent is defined as

$$H = z_{\max} - z_{\min} \quad (10)$$

where $z_{\max}$ and $z_{\min}$ are the maximum and minimum z coordinates of the deposited-atom group.

A more robust measure of the vertical distribution was obtained from the root-mean-square vertical spread of the deposited atoms,

$$R_z = \left[\frac{1}{N_{\text{dep}}} \sum_{i=1}^{N_{\text{dep}}} (z_i - \bar{z})^2 \right]^{1/2} = \sqrt{\langle z^2 \rangle - \langle z \rangle^2} \quad (11)$$

In the present work the averaging is performed over all deposited atoms; therefore R_z is rigorously described as an RMS vertical spread of the deposited atom population, not as a conventional AFM-style surface roughness.

For direct comparison with the conventional MD thin-film roughness definitions used by Hwang et al. [8] and Jing et al. [Z], only exposed surface atoms should be included:

$$R_q = \left[\frac{1}{N_s} \sum_{i=1}^{N_s} (z_i^{\text{surf}} - \bar{z}_s)^2 \right]^{1/2} \quad (12)$$

where N_s is the number of exposed surface atoms and z_i^{surf} is the height of each exposed atom. Equation (12) is recommended for a future surface-only reanalysis of the existing trajectories and should be reported as R_q .

where angle brackets denote averaging over the 300 deposited atoms. R_z is referred to throughout this paper as the RMS vertical spread. It should not be confused with an experimental AFM R_a or R_q value computed relative to a fitted surface profile; rather, it is a direct atomistic measure of how broadly the deposited population is distributed along z .

The average coordination number was calculated using a 3.0 Å neighbor cutoff. Bulk FCC Cu has 12 nearest neighbors, whereas atoms at a free surface necessarily have reduced coordination. For the ultrathin deposited layer in this study, an average coordination near eight is therefore physically plausible and can be used comparatively to assess local packing. The final metric was the average per-atom potential energy of the deposited group. A more negative value generally indicates a more strongly bound local environment within the same potential model, although direct comparisons across different temperatures must be interpreted together with morphology and coordination rather than as a standalone thermodynamic free energy.

$$CN_i = \sum_{j \neq i} \theta(r_c - r_{ij}), \quad \overline{CN} = \frac{1}{N_{\text{dep}}} \sum_i CN_i \quad (13)$$

Here θ is the Heaviside step function and $r_c = 3.0$ Å is the neighbor cutoff used in the current LAMMPS calculation. The mean coordination is evaluated over the deposited atom group.

$$\overline{E}_{\text{pot}} = \frac{1}{N_{\text{dep}}} \sum_{i=1}^{N_{\text{dep}}} E_i^{\text{pot}} \quad (14)$$

The average deposited-atom potential energy is used as a local energetic descriptor. It is not a free energy and should not be used as an absolute thermodynamic ranking across different temperatures.

Trajectories were written every 500 steps and visualized in OVITO. Substrate atoms and deposited atoms were retained as different atom types for visualization only; both types represented Cu and used the same mass and EAM interaction. This color separation enabled the deposition process to be followed from isolated incident atoms through adsorption, lateral redistribution, coalescence, and the final ultrathin film.

2.5 Additional MBE descriptors for structural validation

Two additional descriptors are particularly useful for strengthening the MBE interpretation. First, the radial distribution function (RDF) measures short- and medium-range atomic order and was used by Jing et al. [7] to confirm retention of FCC Cu during deposition and annealing:

$$g(r) = \frac{V}{4\pi r^2 \Delta r N(N-1)} \sum_i n_i(r, r + \Delta r) \quad (15)$$

where $n_i(r, r + \Delta r)$ is the number of neighbors of atom i in a spherical shell of thickness Δr . For FCC Cu, the locations and widths of the first several RDF peaks provide a direct structural check of crystallinity and disorder.

Second, the atomic virial stress can quantify deposition-induced residual stress. A common form is

$$\boldsymbol{\sigma} = \frac{1}{V} \left[\sum_i m_i \mathbf{v}_i \otimes \mathbf{v}_i + \frac{1}{2} \sum_i \sum_{j \neq i} \mathbf{r}_{ij} \otimes \mathbf{f}_{ij} \right] \quad (16)$$

where V is the averaging volume, $\mathbf{v}_i$ is the velocity relative to the center-of-mass motion, $\mathbf{r}_{ij}$ is the pair separation vector, and $\mathbf{f}_{ij}$ is the interatomic force. Hwang et al. [8] used an equivalent atomic-stress formulation to discuss biaxial and normal stress after deposition. Stress was not extracted in the present nine-case dataset and is therefore proposed as an extension rather than reported as a current result.

The temperature dependence of adatom mobility can be interpreted using an Arrhenius-type surface diffusivity relation:

$$D_s = D_0 \exp\left(-\frac{E_m}{k_B T}\right) \quad (17)$$

where D_0 is a prefactor and E_m is an effective surface migration barrier. Equation (17) is used only as a physical interpretation of the observed temperature sensitivity; no diffusion coefficient or migration barrier was fitted from the current trajectories.

3 RESULTS AND DISCUSSION

3.1 Numerical stability and deposition evolution

The corrected Cu(001) model remained stable during the initial equilibration, with all 3456 substrate atoms retained and no lost-atom event. The potential energy remained negative and approximately stationary over the equilibration interval, confirming that the EAM lattice was mechanically stable before deposition. This stability check is important because the initial trial geometry contained duplicate periodic-boundary sites and produced rapidly increasing potential energy and lost atoms. Removing the duplicate boundary sites generated the intended 3456-atom substrate and eliminated the instability.

The time-resolved trajectories show the expected qualitative sequence of atomistic deposition. At early times only a small number of blue deposited atoms are present above or on the red substrate surface. As deposition continues, arriving atoms adsorb at the surface, diffuse or exchange locally, and progressively occupy a larger fraction of the surface. By the final trajectory frame, the deposited atoms form an almost continuous ultrathin layer whose local height varies with processing condition. A representative 300 K, 1 eV trajectory is shown in Figure 2. The early frame demonstrates discrete adsorption events and a largely exposed Cu(001) surface. The final frame shows extensive surface coverage, with deposited atoms distributed across the top plane and locally forming raised regions.

Because the present deposition quantity is only 300 atoms, the simulated structure should be described as an early-stage or ultrathin deposited layer rather than a thick continuous engineering film. Nevertheless, the system contains enough deposited atoms to resolve meaningful differences in vertical distribution and local coordination across the nine cases.

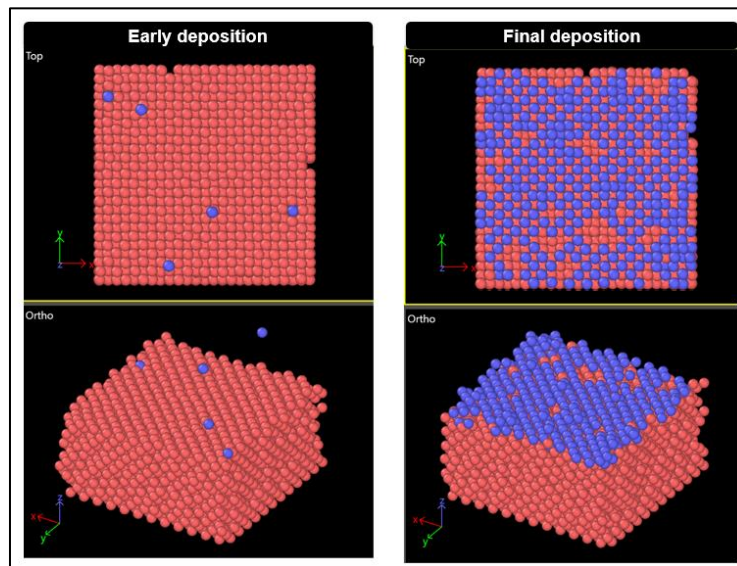


Figure 2: Representative trajectory evolution for the 300 K, 1 eV case. Red atoms are the original Cu substrate and blue atoms are deposited Cu. The early stage contains isolated incident and adsorbed atoms, whereas the final stage shows near-surface coverage and coalescence of the deposited population.

3.2 Final morphology across the temperature-energy matrix

Figure 3 compares the final morphology for all nine combinations of temperature and incident energy. The deposited atoms remain concentrated near the free surface in every case, confirming that the selected energies are in a low-energy deposition regime relative to the tens-of-electron-volt conditions commonly associated with strong sputtering and deep collision cascades [9]. However, the morphology is not identical across the matrix. Both the vertical spread and the occurrence of locally elevated or embedded atoms change with the energy-temperature combination.

At 300 K, the 0.1 eV case produces a relatively narrow deposited population, whereas 1 eV produces a visibly broader height distribution. Increasing the energy to 5 eV reduces the RMS vertical spread relative to the 1 eV case, but also moves the minimum deposited-atom z coordinate closer to the substrate surface plane. At 500 and 700 K, the contrast between 1 and 5 eV becomes stronger. The 1 eV cases show the smallest RMS vertical spreads at these temperatures, while the 5 eV cases show increased height variation. This non-monotonic behavior indicates that the incident-energy effect cannot be represented by a single statement such as 'higher energy always smooths the film.' Instead, the competition between mobility, impact-driven rearrangement, and incipient penetration must be considered.

The final 700 K, 5 eV morphology is particularly important. It combines the largest RMS vertical spread with the highest average coordination number of the entire dataset. This apparently contradictory result shows why morphology and local bonding must be analyzed separately. High energy and high temperature can allow atoms to find more highly coordinated environments while also enabling exchange or penetration events that broaden the vertical distribution of the deposited population.

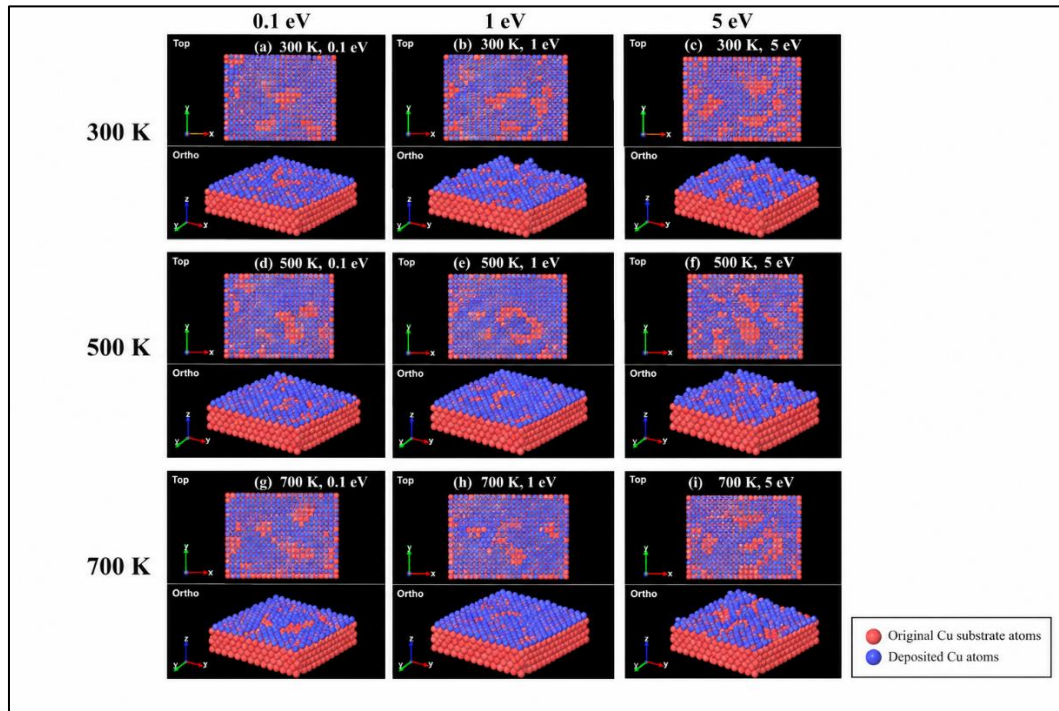


Figure 3: Final OVITO morphologies for the complete 3 x 3 parameter matrix. Rows correspond to 300, 500, and 700 K; columns correspond to 0.1, 1, and 5 eV. Blue atoms are deposited Cu and red atoms are substrate Cu.

Table 2: Final deposited-atom metrics for the nine simulated conditions.

T (K)	E (eV)	$z_{\min}$ (Å)	$z_{\max}$ (Å)	Extent (Å)	RMS spread (Å)	Coord.	PE (eV/atom)
300	0.1	21.531	23.830	2.299	0.658	7.947	-2.943
300	1	21.399	26.995	5.596	0.841	7.967	-2.945
300	5	19.940	23.756	3.816	0.683	8.100	-2.981
500	0.1	21.509	25.322	3.813	0.684	8.013	-2.931
500	1	20.071	24.239	4.168	0.634	7.963	-2.930
500	5	19.949	24.042	4.094	0.889	8.310	-2.976
700	0.1	20.048	24.317	4.270	0.702	8.053	-2.927
700	1	19.988	24.263	4.275	0.629	7.950	-2.924
700	5	18.394	24.208	5.815	0.964	8.700	-3.021

3.3 RMS vertical spread and vertical extent

The RMS vertical spread provides the clearest compact measure of the deposited-layer morphology. At 300 K, R_z increased from 0.658 Å at 0.1 eV to 0.841 Å at 1 eV, then decreased to 0.683 Å at 5 eV. Thus, the 300 K response is non-monotonic, with the intermediate-energy case producing the largest height dispersion. At 500 K, R_z changed from 0.684 Å at 0.1 eV to a minimum of 0.634 Å at 1 eV and then increased strongly to 0.889 Å at 5 eV. The 700 K series showed the same general pattern as 500 K: 0.702 Å at 0.1 eV, a minimum of 0.629 Å at 1 eV, and a maximum of 0.964 Å at 5 eV.

The 500 and 700 K results therefore identify 1 eV as a comparatively smooth condition within the tested range. Relative to 1 eV, increasing the energy to 5 eV raises the RMS spread by about 40% at 500 K and about 53% at 700 K. These

increases are too large to be explained by minor numerical noise and are also consistent with the visibly broader morphology in the trajectory images. The result differs from some prior studies in which roughness decreased monotonically with increasing incident energy over a specified low-energy range [Z]. However, the difference is not necessarily contradictory because roughness trends depend on deposition rate, film thickness, temperature, substrate structure, potential, and the exact metric used. The present simulations use a very short deposition interval and a single deposited population of 300 atoms, so the system is dominated by early-stage adsorption and rearrangement rather than steady-state multilayer growth.

The vertical extent, $z_{\max} - z_{\min}$, is more sensitive to individual outlier atoms than R_z . At 300 K it increases sharply from 2.299 Å at 0.1 eV to 5.596 Å at 1 eV and then falls to 3.816 Å at 5 eV. At 500 K the extent remains within a narrower range of 3.813–4.168 Å. At 700 K, however, the 5 eV case reaches 5.815 Å, the largest value in the entire matrix. The agreement between the high RMS spread and high vertical extent at 700 K, 5 eV indicates that this case contains a genuine broadening of the deposited-atom z distribution rather than only a single isolated high atom.

A further clue comes from $z_{\min}$. The highest substrate atomic plane in the constructed FCC slab lies near 19.88 Å. For most cases the minimum deposited-atom z coordinate remains close to or above this level. At 700 K and 5 eV, $z_{\min}$ decreases to 18.394 Å, placing part of the deposited population below the nominal top substrate plane. This provides atomistic evidence for impact-assisted exchange or shallow penetration at the highest combined temperature and energy used here. Similar energy-dependent exchange and penetration mechanisms have been reported in prior Cu deposition simulations, although the threshold energies depend strongly on the employed potential and model conditions [9].

3.4 Coordination number and deposited-atom potential energy

The average coordination number provides a complementary structural measure. Because the deposited atoms reside at or near a free surface, their coordination is expected to remain below the bulk FCC value of 12. Across the full matrix, the mean coordination varies from 7.95 to 8.70. At 0.1 eV, coordination increases slightly with temperature, from 7.947 at 300 K to 8.013 at 500 K and 8.053 at 700 K. At 1 eV, the values remain essentially unchanged, 7.967, 7.963, and 7.950, indicating that temperature alone does not substantially alter local packing under this moderate impact energy during the short simulated time.

The strongest coordination response occurs at 5 eV. The average coordination increases from 8.10 at 300 K to 8.31 at 500 K and 8.70 at 700 K. The 700 K, 5 eV configuration therefore has approximately 9% higher coordination than the 700 K, 1 eV configuration. This increase indicates that the combined kinetic and thermal energy enables more deposited atoms to occupy locally dense environments. Importantly, the higher coordination does not correspond to a smoother vertical distribution. The same 700 K, 5 eV condition also has the largest RMS spread. This demonstrates a central result of the study: improved local packing and reduced surface-height dispersion are not equivalent objectives.

The average potential energy of the deposited atoms supports this interpretation. At 300 K, the average potential energy changes only slightly between 0.1 and 1 eV, from -2.943 to -2.945 eV/atom, but becomes more negative at 5 eV, -2.981 eV/atom. At 500 K, the values are -2.931, -2.930, and -2.976 eV/atom for 0.1, 1, and 5 eV, respectively. At 700 K, the 5 eV case reaches -3.021 eV/atom, markedly more negative than -2.927 and -2.924 eV/atom at 0.1 and 1 eV. The more negative value is consistent with the higher coordination and suggests that a larger fraction of deposited atoms occupies strongly bonded local environments after the 5 eV impacts.

Potential energy is not a free energy and the simulations are performed at different temperatures; therefore, the values should not be interpreted as a strict thermodynamic ranking of process conditions. Nevertheless, when potential energy, coordination, and morphology are considered together, the data show a coherent pattern. The high-energy, high-temperature condition enhances local bonding and packing but simultaneously broadens the z distribution and promotes shallow penetration. The moderate-energy condition at 500–700 K produces a smoother deposited population but does not maximize coordination. This process-property tradeoff is more informative than identifying a single 'best' condition.

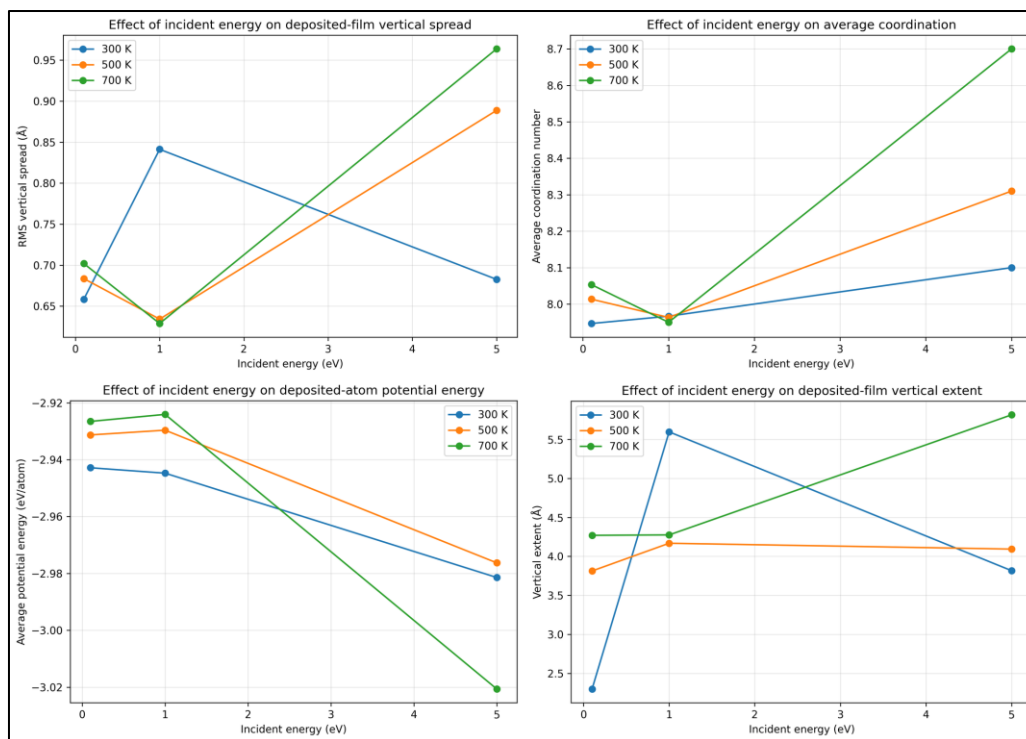


Figure 4: Quantitative dependence of the deposited layer on incident energy and substrate temperature: RMS vertical spread, average coordination number, average deposited-atom potential energy, and vertical extent. Each curve contains the three incident-energy cases for one substrate temperature.

3.5 Comparison with prior atomistic deposition studies

The present results can be placed in context with earlier MD deposition studies, but direct one-to-one agreement should not be expected because deposition rate, substrate orientation, system size, potential, and film thickness differ. Jing et al. reported approximately layer-island growth for Cu on Cu(001) from 1 to 5 eV and increasing surface intermixing at 10 eV [7]. Their findings support the idea that the 1-5 eV range lies near a transition between predominantly adsorptive growth and increasingly impact-assisted rearrangement. In the current simulations, the 5 eV cases show higher coordination and, at 700 K, a lower minimum z coordinate, both of which are consistent with enhanced impact-driven rearrangement before the energy range associated with extensive sputtering is reached.

Gilmore's energetic Cu-on-Cu(001) study explored a substantially higher energy range, 5-80 eV, and reported surface exchange at the low end and progressively deeper penetration and defect formation as energy increased [9]. The present 5 eV cases therefore represent the beginning of the energetic-deposition regime rather than the collision-cascade regime. This distinction is important when interpreting the absence of extensive sputtering or deep defects in the trajectories. The chosen energy matrix is intentionally focused on morphology and early-stage film packing rather than radiation-like damage.

Studies of Cu deposition on dissimilar substrates have also emphasized the non-universality of roughness trends. Hwang et al. observed a minimum roughness at an intermediate incident energy in a Cu cluster-on-Si system [8], whereas Mes-adi et al. reported that incident energy and substrate temperature could reduce roughness in Cu-on-Si simulations [11]. A recent Cu-on-Ta study further showed that deposition temperature can correlate positively with roughness while higher incident energy decreases roughness up to a saturation regime [10]. These differences reinforce the need to treat the present result as a property of the specific Cu-on-Cu(001), short-time, high-flux simulation protocol. The physically significant outcome is not that 1 eV is universally optimal, but that the energy-temperature coupling generates competing trends in roughness, local coordination, and penetration.

The current study also differs from experimental MBE in flux and accessible time scale. Experimental MBE involves a much lower arrival rate and permits adatoms to diffuse over far longer physical times between impacts [1]. The MD deposition rate used here compresses this evolution into tens of picoseconds. Consequently, thermally activated diffusion that would occur between widely separated experimental arrival events is underrepresented, while impact-induced processes are relatively emphasized. The model should therefore be viewed as a controlled atomistic sensitivity study that reveals mechanisms and relative trends.

4 MODEL LIMITATIONS AND RECOMMENDED EXTENSIONS

Several limitations should be considered before using the present trends for process design. First, the deposited amount is 300 atoms, so the simulation represents an ultrathin early-stage film rather than a many-monolayer coating. Surface roughness measured during later steady-state growth may differ because mound coarsening, step-flow processes, defect accumulation, and grain competition are not yet fully developed. Second, the deposition rate is many orders of magnitude larger than experimental MBE flux. This is a standard limitation of classical MD, but it reduces the amount of thermally activated diffusion available between successive impacts.

Third, the present analysis separates substrate and deposited atoms by atom type for tracking purposes even though they are chemically identical Cu atoms. This is useful for computing deposited-group statistics, but after exchange events a deposited atom may move into the substrate while an original substrate atom can move toward the surface. A more complete analysis should therefore supplement the group-based metrics with local structural descriptors that are independent of atom history. Polyhedral template matching, common-neighbor analysis, centrosymmetry parameter, and dislocation extraction in OVITO are appropriate next steps [6]. The current trajectory files already contain per-atom centrosymmetry values, so a follow-up study can quantify the fraction of FCC-like, HCP-like, and disordered environments.

Fourth, the quantity obtained directly from the LAMMPS simulations is the RMS vertical spread of the entire deposited-atom population, R_z , as defined in Eq. (11), rather than the conventional surface-only RMS roughness, R_z , defined in Eq. (12). This distinction is important. This distinction is important because published Cu deposition studies typically evaluate roughness using only the exposed surface atoms [7,8]. Therefore, the current R_z trends are valid as a measure of vertical morphology, but a publication aimed specifically at MBE surface quality should additionally calculate R_q from the topmost or exposed atoms in the final trajectories.

Finally, only one random deposition sequence was used for each condition. Because atom insertion positions are stochastic, repeated simulations with different random seeds would allow error bars to be reported. A practical next-stage design would use three to five independent seeds for each of the nine conditions and then report the mean and standard deviation of roughness, coordination, penetration depth, and potential energy. Additional factors such as deposition rate, incident angle, substrate orientation, and post-deposition annealing can then be introduced through a design-of-experiments framework.

5 CONCLUSIONS

A nine-case molecular dynamics study was carried out to examine Cu thin-film growth under molecular beam epitaxy conditions on Cu(001) as a function of substrate temperature and incident kinetic energy. The model is governed by Newton's equations of motion, the Mishin EAM many-body description of Cu-Cu interactions, controlled beam kinetic energy, and a Langevin substrate thermostat. The corrected simulation contained 3456 substrate atoms and retained all 300 incident atoms in every case. The results identify a non-monotonic morphology response: 1 eV gives the smallest RMS vertical spread at 500 and 700 K, whereas 5 eV increases deposited-atom coordination and lowers the average potential energy while simultaneously increasing vertical dispersion. The distinction between the present deposited-atom RMS vertical spread and a true surface-only R_q roughness is explicitly established. The present atomistic model represents the essential surface-growth stage of molecular beam epitaxy by introducing energetic Cu atoms through a vacuum region toward a temperature-controlled Cu(001) substrate, thereby resolving adsorption, surface migration, local rearrangement, and film formation as functions of incident kinetic energy and substrate temperature. Future computational work using exposed-atom roughness, RDF, PTM/CNA, virial stress, and repeated random seeds could provide a more comprehensive description of film morphology, local crystallinity, residual stress, and the statistical reproducibility of the simulated MBE growth behavior.

STATEMENTS ON COMPLIANCE WITH ETHICAL STANDARDS

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Disclosure of conflict of interest

The author declares no conflicts of interest regarding this manuscript.

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