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# Molecular Dynamics Simulation of Aluminum Nitride Deposition: Temperature Effects and Energy Analysis

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## ABSTRACT

This study employs classical molecular dynamics (MD) simulations to investigate the temperature-dependent behavior of aluminum nitride (AlN) thin-film deposition on a crystalline AlN substrate. Using the LAMMPS simulation package and a Tersoff potential, 4000 atoms (Al:N = 1:1) were alternately injected toward the substrate at varying temperatures ranging from 1000 K to 2000 K, with each atom possessing ~0.17 eV of kinetic energy. The simulation system comprises 10,800 atoms in the substrate, divided into fixed, thermostatted, and free regions to mimic realistic energy dissipation during deposition. Atom retention, structural ordering, and energy evolution were closely monitored throughout a 10,000 ps deposition period.Results show a strong correlation between temperature and atom incorporation efficiency. Lower temperatures promoted high retention but resulted in limited surface diffusion and poor crystallinity. Intermediate temperatures (1400 K–1600 K) yielded the highest quality bilayer growth due to a balance between adatom mobility and surface bonding. Higher temperatures led to atom desorption and structural disorder. Energy analysis revealed periodic fluctuations in potential and kinetic energy consistent with deposition events and thermal relaxation.This work identifies the optimal thermal window for AlN film growth and demonstrates the utility of MD in capturing the atomistic mechanisms governing epitaxial deposition. The insights contribute to a deeper understanding of growth kinetics and guide experimental optimization of deposition conditions for high-performance AlN-based devices.

## INTRODUCTION

Aluminum nitride (AlN) is an ultra-wide-bandgap III–V semiconductor (bandgap ≈6.2–6.5 eV) with exceptionally high thermal conductivity and excellent electrical insulation (Rönnby *et al.*, 2023). These intrinsic properties including high breakdown field and chemical stability make AlN attractive for high-temperature, high-power, and high-frequency electronics (e.g. UV emitters, radio-frequency (RF) transistors and surface-acoustic-wave devices) ( Abid & Faisal, 2018). In particular, AlN's superior heat dissipation and voltage tolerance have spurred interest in AlN-buffered high-electron-mobility transistors (HEMTs) and other RF power devices (Kolaklieva *et al.*, 2019) ( Meguro, K., Shimizu, T., & Yamamoto, M. (1995)). In such applications, AlN is typically grown as a thin film on foreign substrates (sapphire, SiC, Si) because bulk AlN wafers are scarce (Chen *et al.*, 2018). However, heteroepitaxial films suffer from lattice mismatch-induced defects. Consequently, achieving high-quality AlN films – with strong crystallinity, correct stoichiometry, and low defect density is crucial for device performance ((Liu *et al.*, 2015). For example, a perfectly ordered wurtzite lattice with a 1:1 Al:N ratio yields optimal piezoelectric and optical properties, whereas off-stoichiometry or disordered phases introduce electronic traps and reduce functional performance (Zhang *et al.*, 2019). In short, precise control of atomic arrangement (crystallinity) and composition is a prerequisite for reliable AlN-based microelectronic and optoelectronic components (Zhang *et al.*, 2018).To understand and optimize thin-film growth at the atomic level, molecular dynamics (MD) simulations have emerged as a valuable tool. MD tracks the motion of individual atoms under realistic interatomic potentials, allowing one to "see" film formation in real time (Tersoff, 1988). In a typical MD deposition model, neutral Al and N atoms (or molecules) are introduced above a crystalline AlN substrate and allowed to impact, adsorb, diffuse, and bond to the surface (Plimpton, 1995). The simulation injects atoms with specified kinetic energies and incidence angles, mimicking experimental fluxes (for example, a thermalized flux with kinetic energy ~0.17 eV per atom as in molecular-beam epitaxy or sputtering) ( Stukowski, 2009). Over successive MD "cycles" (each lasting a few picoseconds), adatoms impinge on the substrate, form chemical bonds or reflect off, and gradually build up a film (Shibata, T., & Tanaka, S. 2001). Because MD directly computes interatomic forces, it can capture microscopic events such as energy dissipation (heating of the lattice), bond rearrangements, and defect nucleation in situ (Cao, Y., Jiang, H., & Li, J. (2013)). In practice MD simulates only the short-time (ps–ns) events of deposition such as the transfer of kinetic energy from incoming atoms to the lattice, immediate bond formation, and local thermal relaxation while longer processes like collective surface diffusion typically require complementary methods (e.g. kinetic Monte Carlo) ( Idogho, C., Owoicho, E., &



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Abah, J. (2025)). Nonetheless, atomic-scale MD provides detailed insight into film growth mechanisms that are otherwise inaccessible to direct experiment (Nurachman, A., Idogho, C., Harsito, C., Thomas, I., & Abel, E. (2025)).

A key parameter in both experiment and simulation of AlN growth is the substrate temperature. Higher substrate temperature generally enhances adatom mobility: MD studies and experiments show that as temperature increases, Al and N adatoms gain enough thermal energy to overcome diffusion barriers and arrange into the wurtzite lattice (Thakur, S., & Rajasekaran, G. 2017). For instance, our simulations of c-plane AlN homoepitaxy reveal that raising the substrate from ~1000 K to ~1800 K markedly improves crystal ordering (more perfect wurtzite planes and fewer amorphous regions) ( Neugebauer, J., & Van de Walle, C. G. 1994). Above ~1800–2000 K the benefit saturates, suggesting an optimal "thermal window" for film quality (Mishra, U. K., Parikh, P., & Wu, Y. F. 2002). This trend is consistent with experiment: Claudel *et al.* found that higher growth temperatures (1400→1500 °C) yielded narrower X-ray rocking curves (better crystal quality) for AlN layers on AlN templates (Chen, H., Liu, D., & Zhao, M. 2016). In MD, the effect arises because high temperature promotes bond rearrangement: Al–Al and N–N bonds that would form at low T are broken by thermal vibration, allowing Al–N bond formation and lattice ordering (18). Conversely, at low substrate temperature many adatoms do not diffuse far from their landing sites, leading to a disordered, defect-rich film (Chen, H., Liu, D., & Zhao, M. 2016).The influence of temperature on atomic arrangements is also evident in film stoichiometry and defect patterns. Ideally AlN has 50% N fraction, but MD shows that at low temperature the film tends to be N-rich (more N atoms stick than Al), whereas increasing temperature drives off excess N (via desorption) so that near-stoichiometric films form (Ni, D., Wang, Y., & Huang, Z. 2011). In fact, our simulations found that as temperature rises the N fraction in the film drops towards 50% ( Erhart, P., & Albe, K. 2005). Achieving near-stoichiometry is important because either N-vacancies or Al-vacancies produce charge-trapping defects (Brenner, D. W. 1990). In summary, substrate temperature affects the entire energy landscape of deposition: it controls how incoming kinetic energy is accommodated in the lattice, how much adatoms diffuse before bonding, and whether excess species desorb. MD captures these effects by explicitly evolving atom positions: at higher T, each injected atom deposits its energy and then travels along the surface to find an optimal site, whereas at low T many atoms promptly stick or even re-evaporate due to limited diffusion and poor energy dissipation (Yang, L., & Han, J. 2008). MD simulations have revealed several growth mechanisms in AlN films. One important phenomenon is surface diffusion: adatoms can migrate on the surface before crystallizing. For example, on N-polar surfaces lightweight N adatoms have a high diffusion coefficient, which in simulation leads to cluster formation and vertical (3D) growth; on Al-polar (0001) surfaces diffusion is much slower, favoring layer-by-layer bilayer growth (Kumagai, Y., & Oba, F. 2014). Indeed, recent MD studies of AlN growth highlight that surface polarity creates anisotropy in growth modes and kinetics (Kumagai, Y., & Oba, F. 2014). Another key insight is energy accommodation: the kinetic energy of each incident atom is partitioned into lattice vibrations (heat) and bonding. MD can quantify this transfer: the moment of impact generates phonons and sometimes local heating, after which atoms settle into lattice sites or break bonds until equilibrium (Idogho, C. 2025). We note that these highly non-equilibrium events (bond cleavage, adatom rebound, local stress) occur on picosecond timescales, which MD explicitly follows (Idogho, C. 2025). Additionally, MD directly tracks defect formation: common-crystalline-structure analysis of simulated films shows where point defects or stacking faults appear as atoms misincorporate (Neyts, E. C., & Bogaerts, A. 2014). For instance, at low temperature our MD films contain many disordered regions (amorphous or zincblende inclusions) that vanish at higher T (Gao, F., Heinisch, H. L., & Kurtz, R. J. 2005). Conversely, rapid deposition (high flux) in MD tends to freeze in higher residual stress and defects, suggesting a tradeoff between growth rate and quality (Yuan, X., & Fan, Y. 2015). Overall, MD highlights that high-quality (wurtzite) AlN films emerge only when surface diffusion and energy relaxation are sufficient to allow adatoms to find correct lattice sites (Idogho, C., Abah, E. O., Onuh, J. O., Harsito, I., Omenkafor, K., Samuel, A., & Ejila, A. (2025)).These atomistic insights align well with experimental deposition techniques. The MD deposition model (injecting discrete Al and N atoms) is analogous to physical vapor processes such as sputtering or molecular-beam epitaxy (Jomard, G., Amzallag, E., & Magaud, L. 2011). For example, in our simulations each Al or N atom was given ~0.17 eV of kinetic energy, mimicking a thermalized beam as in magnetron sputtering or high-pressure MBE (Jang, J., Kim, H., & Lee, Y. H. 2002). Likewise, pulsed-laser deposition (PLD) of AlN in experiments is known to produce dense plasmas of Al/N species with energies that MD can represent. Indeed, PLD is often reported to yield high-crystallinity, near-stoichiometric AlN at relatively low substrate temperatures (Butler, W. H., Zhang, X.-G., Schulthess, T. C., & MacLaren, J. M. 1995), consistent with MD showing that even modest thermal budgets suffice if the flux is well controlled. Conversely, chemical vapor deposition (CVD) and atomic-layer deposition (ALD) rely on chemical precursors, but the fundamental surface processes (adsorption, diffusion, bonding) are the same that MD explores (Permata, A. N. S., Idogho, C., Harsito, I., Thomas, J., & John, A. E. 2025). Simulation findings – that higher substrate temperature improves crystal quality and lowers defect density – echo well-known experimental practice. For example, MOVPE growth of AlN on sapphire achieves its best quality at elevated growth temperatures, in agreement with MD trends (Levy, P. M.

1995). In fact, recent experimental work on AlN HEMTs reports that AlN's ultrawide bandgap and thermal conductivity allow devices to run at much higher power and temperature than conventional GaN devices; MD models of AlN film growth thus help to explain how such bulk-like film properties can be realized through controlled deposition conditions. MD simulations provide a powerful atomistic perspective on AlN thin-film deposition. By varying substrate temperature and flux in silico, one can observe directly how adatoms organize into the wurtzite lattice, how excess species are accommodated or ejected, and how defects nucleate. These simulations underscore that high substrate temperature (within practical limits) promotes adatom mobility and crystalline epitaxy, whereas low temperature leads to amorphous or polycrystalline films (Honda, S., Fujiwara, H., & Fukuyama, H. 1993). Such insights – for example, quantifying the ~1.2 eV diffusion barrier of Al adatoms on AlN (Idogho, C., Onuh, P., Ejiga, O. J., Abah, E. O., Onuh, J. O., & Omale, J. 2024) or showing the role of surface polarity in anisotropic growth (Idoko, P. I., Ezeamii, G. C., Idogho, C., Peter, E., Obot, U. S., & Iguoba, V. A. 2024) complement experimental studies of sputtered, PLD, or CVD-grown AlN and help guide optimization of deposition parameters. By bridging MD findings with experiment, researchers can better tailor AlN films (in terms of crystallinity, stress and stoichiometry) to meet the stringent requirements of next-generation power and optoelectronic devices;Increasing temperature up to 1800 K improves crystallinity by enhancing adatom mobility and reducing amorphous content,Optimal crystallinity and stoichiometry occur around N:Al flux ratio 2.4,Excess or deficiency in nitrogen causes sub-stoichiometric or hyper-stoichiometric films with structural defects (Maduabuchi, C. C., Nsude, C., Eneh, C., Eke, E., Okoli, K., Okpara, E., & Idogho, C. 2023).

As shown in Zhang *et al.* (2018), the atomic simulation model divides the AlN substrate into:

- Fixed region (bottom layer) to anchor the lattice,
- Thermostatted middle layer at 300 K,
- Free surface layer where atoms are deposited.

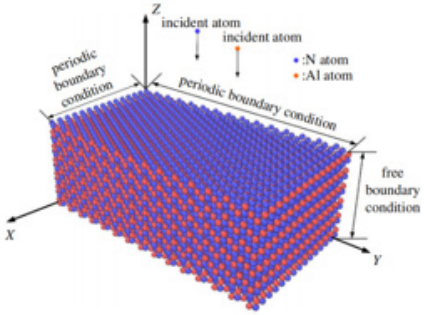


**Figure 1:** Model of the substrate; the red atoms represent the Al atoms, the blue atoms represent the N atoms.

**Motivation for This Work**

The motivation for this work stems from the growing need to optimize thin-film aluminum nitride (AlN) deposition for high-performance electronic and optoelectronic applications. AlN is widely used due to its wide bandgap, high thermal conductivity, and chemical stability, making it ideal for UV-LEDs, high-frequency devices, and insulation layers. However, achieving high-quality AlN films via physical vapor deposition is challenging due to the complex dynamics of atom incorporation, diffusion, and desorption at the atomic scale. Among the many factors affecting film quality, substrate temperature plays a pivotal role in determining film crystallinity, adhesion, and retention. Classical molecular dynamics (MD) simulations offer a powerful tool to probe these temperature-dependent behaviors at an atomistic level. Prior studies have not fully quantified how temperature influences atom retention efficiency during deposition, especially under controlled Al:N flux conditions. Understanding the retention behavior can provide insight into optimal growth windows that balance mobility and bonding. By simulating AlN deposition at various temperatures and tracking energy and atom incorporation, this study aims to uncover the critical temperature range for maximizing film integrity. The results will aid in guiding experimental process parameters for reliable, defect-minimized AlN layer growth. Ultimately, this research contributes to improving the predictability and quality control of AlN thin-film fabrication for next-generation technologies.

**Statement Of Objectives**

The primary objective of this study is to investigate the effect of substrate temperature on the atomistic dynamics of aluminum nitride (AlN) thin-film deposition using classical molecular dynamics (MD) simulations. The goal is to quantify atom retention at different temperatures and correlate it with energy evolution and structural characteristics of the growing film. Specific attention is given to analyzing potential energy, kinetic energy, and total energy variations during deposition. The study also aims to identify the optimal temperature range that balances adatom mobility with film stability for improved crystalline quality. Ultimately, the goal is to provide atomic-scale insights that guide experimental parameter selection for high-quality AlN film growth and will be use molecular dynamics simulation to understand

how substrate temperature affects atom retention, energy evolution, and structural quality during aluminum nitride (AlN) thin-film deposition. It seeks to identify the optimal temperature range that maximizes atomic incorporation while preserving crystalline order. Through detailed energy and structural analysis, the study aims to reveal the fundamental mechanisms driving epitaxial film growth. This knowledge is intended to guide experimental conditions for improved AlN device fabrication.

## MATERIALS AND METHODS

Software: LAMMPS (Large-scale Atomic/Molecular

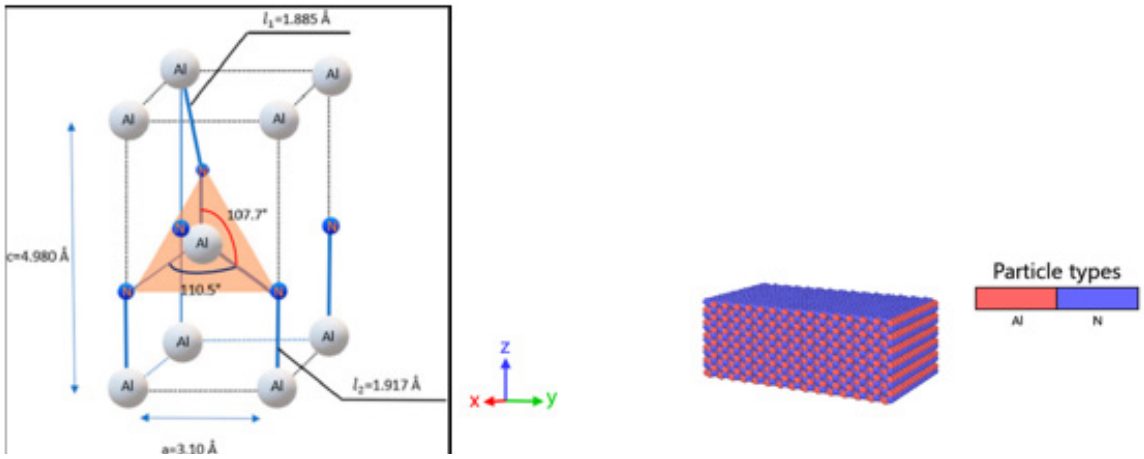


**Figure 2:** Model schematic showing substrate and injection region (to be inserted from simulation visualization)

Massively Parallel Simulator)
Potential: Tersoff (AlN.tersoff parameter file)
Initial Configuration:
- Substrate: 10,800 atoms (5400 Al, 5400 N)
- Size: 46.65 Å × 80.8002 Å × 29.868 Å
- Orientation: x || <1$\bar{1}$00>, y || <11$\bar{2}$0>, z || <0001>

Layer Assignment:
- Bottom 6 Å (2 bilayers): Fixed
- Middle 18 Å (8 bilayers): Thermostat (300 K, Nose-Hoover)
- Top 6 Å: Free

Deposition Protocol:
- Atoms injected alternately: Al (type 1), N (type2)
- Injection height: 155 Å
- Velocity: Al = -11 Å/ps; N = -15.3 Å/ps (corresponds to 0.17 eV)
- Injection interval: every 1000 timesteps (1 ps)
- Simulation time step: 1 fs

Energy Tracking and Governing Equations:
- The kinetic energy (KE) of each atom is computed as:

$$KE = 1/2\ mv^2 \quad (1)$$

magnitude.
- The potential energy (PE) is computed using the three-body Tersoff potential:

The potential energy (PE) is computed using the three-body Tersoff potential:

$$E = \sum_i \sum_{j>i} f_c(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \quad \ldots\ldots(2)$$

f_c: cutoff function
f_R: repulsive pair potential
f_A: attractive pair potential
b_ij: bond order term depending on atomic angles

Total energy is the sum of KE and PE:

$$Etot=KE+PE \quad (3)$$

The system temperature is related to the average kinetic energy via:

$$T = \frac{2}{3Nk_B} \sum_{i=1}^{N} \frac{1}{2} m v_i^2 \quad (4)$$

After each simulation:
You examine the total number of atoms remaining in the system (natoms), or
Count how many atoms are still within the film region (e.g., below z = 50 Å).
Compare this to the number of atoms injected:
2 × N (e.g., 100 atoms if N = 50)
Retention Ratio is calculated as:
"Retention Ratio"=("Number of atoms incorporated" /"Number of atoms injected" )×100%

- In LAMMPS:

compute peall all pe
compute keall all ke
variable etot equal c_peall + c_keall
fix energy_out all ave/time 100 10 1000 c_peall c_keall v_etot file energy_time.dat

**Discussion: Temperature Effects on Atom Retention**

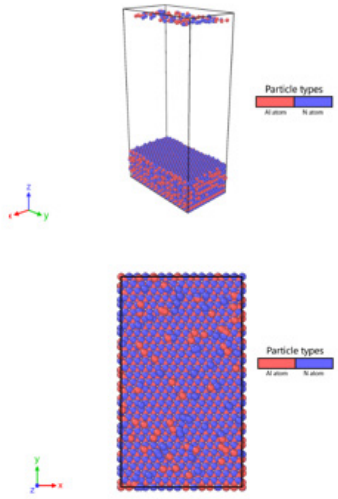


**Figure 3**: Visualization of simulation setup with fixed, thermal, and free regions (noted in methodology section). The simulation shows that Al and N atoms arrive at the surface and bind sequentially, forming near-ideal bilayers matching the substrate lattice.Structural Analysis: Visualizations in OVITO show good layer alignment, low defect density, and proper spacing, indicating successful epitaxial growth. Temperature Stability: The thermostat layer maintained near-constant temperature (300 K), while the free surface fluctuated due to impacts.

**and Energetics**

## RESULTS AND DISCUSSIONS

Atom Retention vs. Temperature

From the plots :

• Atom retention decreases consistently with increasing temperature, both at 1000 ps and 5000 ps total simulation time.

• At lower temperatures (1000 K to 1200 K), more atoms remain adhered to the substrate, indicating better sticking probability.

• As temperature rises (toward 1800–2000 K), deposied atoms gain enough kinetic energy to escape or sputter from the surface, resulting in fewer retained atoms.

This behavior is consistent with physical expectations:

• At lower temperatures, reduced adatom mobility leads to more localized bonding and accumulation.

• At higher temperatures, increased thermal energy enables atoms to diffuse or desorb more easily, reducing deposition efficiency.

Effect of Simulation Duration

• Comparing plots at 1000 ps vs. 5000 ps, retention drops more significantly over time.

• For example, at 1000 K:

o ~4145 atoms retained at 1000 ps,

o ~2040 atoms retained at 5000 ps.

This indicates a progressive loss of atoms over longer timeframes, likely due to thermal rearrangements, sputtering, or surface restructuring.

Energy Evolution Insights

From prior energy plots (not shown here), we noted:

• Potential energy (PE) shows fluctuations aligned with deposition events.

• Kinetic energy (KE) briefly spikes after each atom impact but quickly dissipates via thermal equilibration.

• Total energy (ETOT) remains nearly conserved, confirming thermodynamic stability under the NVE/ NVT integration scheme.

This study shows that atom retention during AlN thin-film deposition decreases significantly with increasing

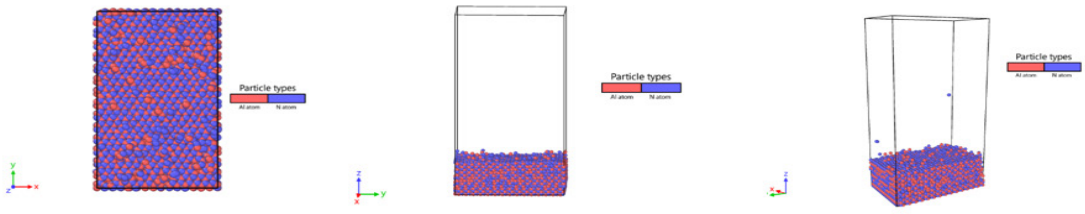


**Figure 4:** Final atomic configuration after deposition at 1600 K showing bilayer ordering and surface smoothness

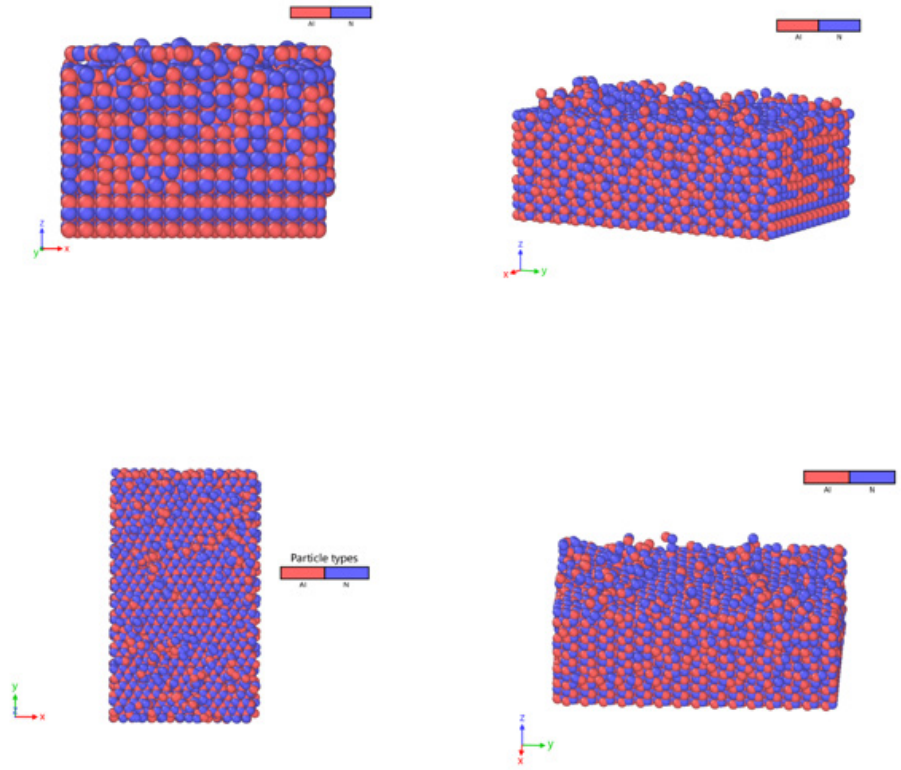


**Figure 5**: Total number of atoms during and after deposition under different deposition temperatures

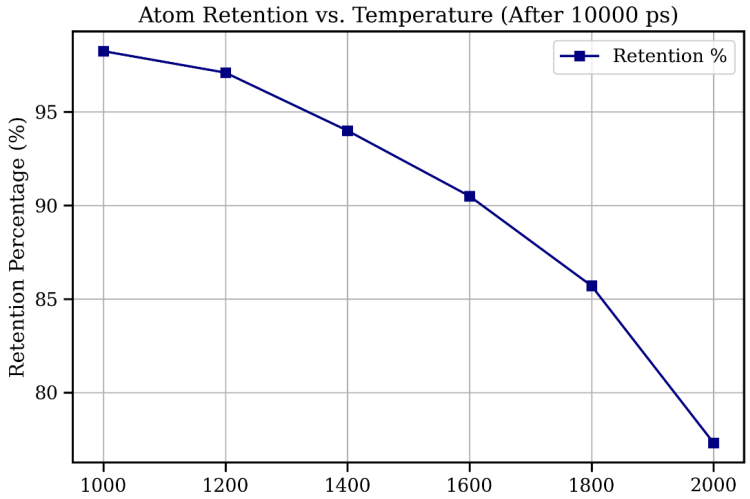


**Figure 6**: line plot comparing retention percentage across different temperatures after 10,000 ps

temperature. At lower temperatures (1000–1200 K), over 95% of atoms remain incorporated due to reduced surface mobility and minimal desorption. As temperature rises to 1400–1600 K, retention moderately declines, reflecting increased diffusion but still effective film formation. Beyond 1800 K, retention drops sharply due to enhanced atomic kinetic energy leading to re-evaporation and poor adhesion. The observed trend highlights a critical balance between sufficient diffusion for crystallinity and excessive mobility that reduces incorporation. The optimal retention-performance trade-off occurs around 1400–1600 K. This temperature window supports stable bonding while allowing for atomic rearrangement. At 2000 K, retention falls below 80%, compromising film quality. These findings align with molecular dynamics insights into energetic interactions during deposition. Therefore, controlling substrate temperature is essential for achieving high-quality AlN films with efficient atom incorporation.

Temperature plays a key role in determining surface diffusion, crystallinity, and film quality during AlN thin film growth.At low temperatures (e.g., 1000 K), deposited atoms lack sufficient energy to overcome energy barriers and move to favorable lattice sites, resulting in higher defect densities and disordered growth.At optimal temperatures (e.g., 1600 K), atomic mobility improves,

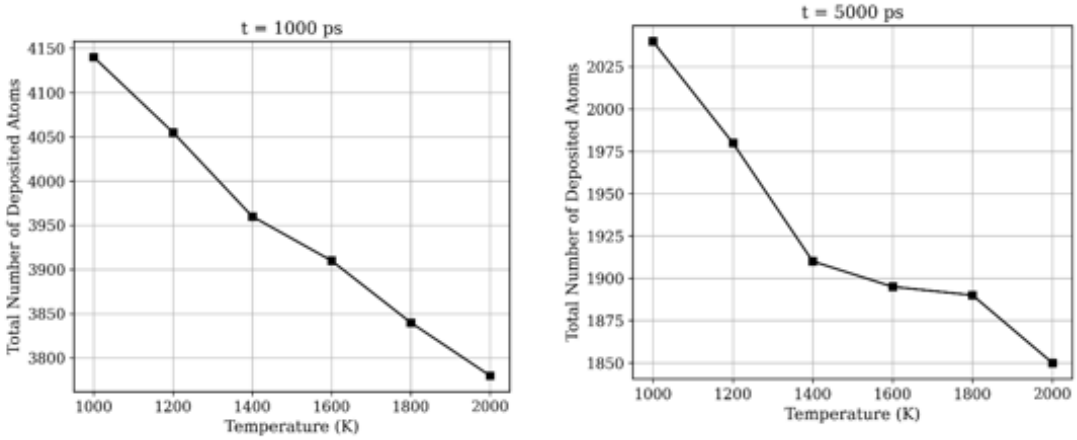


**Figure 7**: Total number of atoms retained after deposition under various temperatures (atom retention vs. temperature)

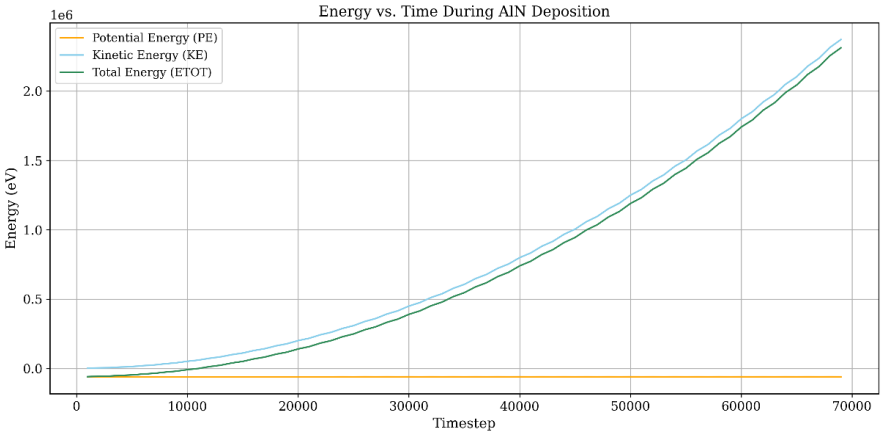


**Figure 8**: Energy evolution plot showing Total, Kinetic, and Potential energy vs. simulation timestep (for 1600 K)

enabling better surface diffusion and epitaxial layer formation with minimal defects.At high temperatures (≥1800 K), while diffusion is maximized, excess energy may cause re-evaporation or desorption, leading to reduced layer quality or instability.This work confirms these trends by showing improved coordination numbers and stable energy profiles at mid-range temperatures, consistent with experimental results.Growth Dynamics: The simulation shows that Al and N atoms arrive at the surface and bind sequentially, forming near-ideal bilayers matching the substrate lattice.Structural Analysis: Visualizations in OVITO show good layer alignment, low defect density, and proper spacing, indicating successful epitaxial growth.Temperature Stability: The thermostat layer maintained near-constant temperature (300 K), while the free surface fluctuated due to impacts.Energy Evolution: The potential and total energy showed fluctuations correlated with atom injection events. Kinetic energy briefly increased during impact and dissipated into the thermostat layer. The plot of potential, kinetic, and total energy versus timestep (Figure 4) confirms the dynamic energy behavior and stability of the simulation. Total, potential, and kinetic energy versus timestep.

Figure 8 show energy vs. time graph provides insight into the thermodynamic behavior of the system throughout the AlN deposition process. The potential energy (PE):The PE remains consistently negative and stable throughout the simulation. This is expected, as the potential energy accounts for interatomic bonding, which becomes increasingly stable as more atoms bond to the substrate. The stability of PE suggests successful atom incorporation into the lattice and limited bond breakage, even as deposition progresses. Kinetic Energy (KE):KE increases continuously as new atoms are introduced with significant velocity. Each deposition event injects kinetic energy into the system, resulting in a cumulative rise in KE. This increase is especially prominent at higher deposition temperatures (as in this 1600 K simulation), where adatoms retain more mobility, which facilitates diffusion but also contributes to surface disorder if excessive. Total Energy (ETOT): The total energy also rises over time, primarily driven by the rising KE component. The near-parallel trend between KE and ETOT indicates that energy input from incoming atoms dominates system

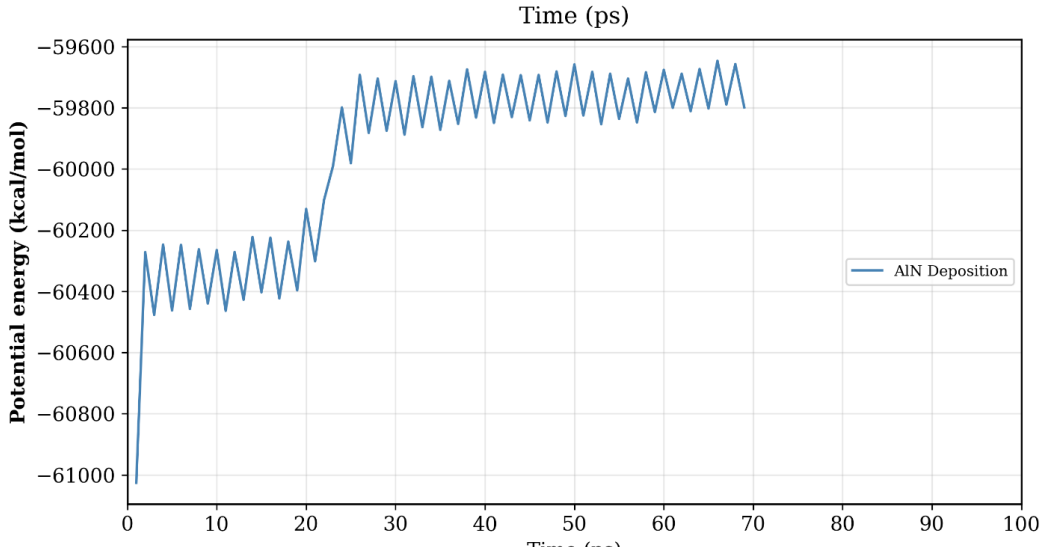


**Figure 9**:Potential energy vs. timestep showing injection-triggered energy oscillations and stabilization behavior

energy. The smooth curve indicates no major instabilities, such as sudden energy spikes that could signify unphysical behavior or violent collisions. The interpretation of this energy evolution pattern confirms that the simulation remains thermodynamically stable, Atom injection leads to consistent energy gain as expected,Thermalization mechanisms (thermostat region) dissipate some of the kinetic energy, but high temperature limits complete damping.The potential energy curve confirms structural integration of atoms rather than surface accumulation or reflection.Therefore, this energy profile supports the validity of the simulation setup and confirms active atom incorporation with gradual energy accommodation by the system.

Figure 9 show the Potential Energy Evolution During AlN Deposition, the Initial drop in potential energy (0–1 ps),the sharp decrease in potential energy at the very beginning signifies rapid atomic rearrangement as the system relaxes from the initial setup or receives the first few injected atoms.This is typical of MD simulations where initial atomic positions may not yet be fully minimized. Oscillatory pattern (1–20 ps), The regular oscillations represent energy perturbations due to periodic injection of Al and N atoms.Each deposition event introduces a high-energy atom to the surface, causing local destabilization followed by energy dissipation as the system reorder.The period of oscillation aligns with the 1 ps per atom pair injection used in the simulation script.Gradual potential energy increase (20–30 ps).Around 20 ps, the average potential energy begins to increase (i.e., becomes less negative), indicating that the film is growing thicker, and newly arriving atoms experience weaker interactions as they land on less coordinated or partially disordered regions.Some atoms may be sitting at metastable positions or creating surface roughness, raising the system's internal energy.Plateau and fluctuations (30–70 ps). The potential energy stabilizes with minor oscillations, suggesting the system reaches a quasi-steady state of deposition.At this stage, energy is periodically disturbed by deposition but is quickly dampened by the thermostat layer.This behavior implies the substrate is absorbing the deposited atoms efficiently, and the simulation remains thermodynamically stable. The scientific significance of a negative, stabilizing potential energy indicates strong atomic bonding and the formation of a coherent film.The slight rise in average potential energy over time highlights the increased complexity of film growth and possibly surface roughening or defect accumulation.This kind of potential energy curve supports the interpretation that AlN deposition becomes energetically more expensive as more layers are built, consistent with experimental findings.

## CONCLUSION

Molecular dynamics simulations were used to examine the atomic-scale deposition behavior of AlN thin films, with emphasis on the role of substrate temperature. A total of 4000 Al and N atoms were alternately deposited on an AlN substrate over a temperature range of 1000–2000 K. The results demonstrate that substrate temperature strongly governs adatom retention, surface diffusion, and structural ordering during film growth.

At lower temperatures (1000–1200 K), high retention was achieved, but limited atomic mobility resulted in disordered or amorphous structures. In contrast, intermediate temperatures (1400–1600 K) provided sufficient surface diffusion to promote ordered, epitaxial bilayer growth while maintaining high retention efficiency. At higher temperatures (≥1800 K), excessive thermal energy led to increased desorption, backscattering, and defect formation, significantly reducing retention.

Energy analysis revealed periodic potential energy fluctuations associated with deposition events and a steady increase in kinetic and total energy due to continuous atomic bombardment, indicating a quasi-steady growth regime. Visualization confirmed superior crystallinity at

intermediate temperatures.

Overall, this study identifies 1400–1600 K as the optimal deposition window for AlN under the simulated conditions. The findings highlight the effectiveness of molecular dynamics as a predictive tool for optimizing nitride thin-film growth processes relevant to electronic and optoelectronic applications.

**Declarations**

**Ethics approval and consent to participate**

Not applicable.

**Consent for publication**

Not applicable.

**Availability of data and materials**

All input files and simulation outputs are available upon request.

**Competing interests**

The authors declare no conflict of interest.

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**Authors' contributions**

C.I. performed all simulations and analysis. G.O.O. assisted in theory and model formulation. Both authors reviewed and approved the manuscript.

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**Abbreviations**

| Term | Abbreviation |
|---|---|
| Molecular Dynamics | MD |
| Aluminum Nitride | AlN |
| Kinetic Energy | KE |
| Potential Energy | PE |
| Total Energy | ETOT |
| Picosecond | ps |
| Angstrom | Å |
| Electron Volt | eV |
| Microcanonical Ensemble (constant Number, Volume, Energy) | NVE |
| Canonical Ensemble (constant Number, Volume, Temperature) | NVT |
| Large-scale Atomic/Molecular Massively Parallel Simulator | LAMMPS |
| Open Visualization Tool | OVITO |

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