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ORIGINAL ARTICLE

Thermal Evaporation of Graphite on Silicon: A Molecular Dynamics Simulation

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ABSTRACT – Silicon, a ubiquitous element in modern electronics, underpins the operation of countless devices due to its unique semiconducting properties. However, as device dimensions shrink to the nanoscale, silicon-based devices face limitations such as increased power consumption and decreased performance. Coating silicon with graphite is aimed to improve the device's performance and extend the limits of silicon's performance. Conducting experimental work involving graphite for thin coatings is a resource-intensive process. Hence, molecular dynamics (MD) simulation is necessary to illuminate the evaporation and coating mechanisms at the atomic scale, serving as a valuable tool for experimental design. These molecular dynamics simulations have elucidated the intricate relationship between temperature and deposition time in governing the quantity and spatial distribution of carbon atoms on a silicon substrate. Within a 300 picosecond deposition interval, a non-linear correlation between temperature and carbon deposition is observed, indicating that the allotted time is insufficient for complete atomic diffusion and homogeneous distribution. At elevated temperatures, carbon atoms accumulate, impeding the diffusion of subsequent atoms. Conversely, a 600 picoseconds deposition period reveals a direct proportionality between temperature and carbon deposition, attributed to the enhanced mobility of carbon atoms, facilitating their dispersion and creation of vacancies within the substrate.

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INTRODUCTION

Due to its favorable semi-conductive characteristics, including high voltage and thermal conductivity, silicon (Si) is frequently employed in micro-electromechanical systems (MEMS) and nano-electrical systems, such as semiconductors. However, silicon is prone to facile oxidation, corrosion, and degradation. To address these issues, nanotechnology has introduced the application of coatings on silicon, such as carbon (C) or graphite, which can form a SiC layer on the silicon substrate. SiC offers notable advantages in terms of mechanical resistance, electrical stability, radiation resistance, and high-temperature endurance. Empirical investigations have demonstrated that the SiC layer can withstand pressures up to 0.15–0.23 MPa and temperatures up to 400°C [1]. The utilization of carbon-coated silicon substrates has been longstanding, with Nishino pioneering the application of the chemical vapor deposition (CVD) method in 1983 [2].

In 2010, Prskalo et al. [3] conducted SiC coating using molecular dynamics. In their research, they performed deposition using the sputtering method to apply SiC on a Si substrate with argon (Ar) using the Tersoff potential—the results of this SiC sputtering aimed to determine the energy function of Ar. The obtained values were found suitable when the results were compared with the experiment. Additionally, the application of carbon coating to a layer was experimentally carried out by Zhang et al. in 2020 [4], [5]. In their study, Zhang achieved a graphite purity of 99.99% on a 150 μm thick nickel (Ni) substrate, with a temperature treatment around 1100°C to 1400°C [4]. In a previous study, Nishino [6] utilized sputtering as the deposition method to simulate a SiC coating. In contrast, Zhang employed evaporation to coat a metal substrate with 99.99% pure carbon [4]. The arrangement of carbon atoms significantly influences material properties. Highly crystalline graphitic carbon coatings offer superior mechanical strength and electrical conductivity compared to amorphous coatings [7]. Given these considerations, graphite was chosen as the precursor material for silicon coating.

In this study, molecular dynamics simulations are employed to provide atomic-level details of the evaporation and coating processes. This computational approach is expected to significantly enhance the efficiency and effectiveness of experimental design.

EXPERIMENTAL METHOD

A 3D coating and coated material model will be constructed using large-scale atomic/molecular massively parallel simulator (LAMMPS) simulator [8]. The initial simulation box size (see Figure 1) is 20a × 20a × 50a (a

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= 2.85 Å, lattice constant of face-centered cubic [FCC] silicon structure), resulting in a box size of 57 × 57 ×142.5 in angstrom units (metal units) with periodic x and y coordinates, while the z coordinate remains fixed. The height of the silicon atoms group (z coordinate) is 57 Å, and the carbon deposited position is 136.8 Å, resulting in 79.8 Å between the silicon and graphite. The model comprises 32,800 silicon atoms and 15,000 atoms of graphite.

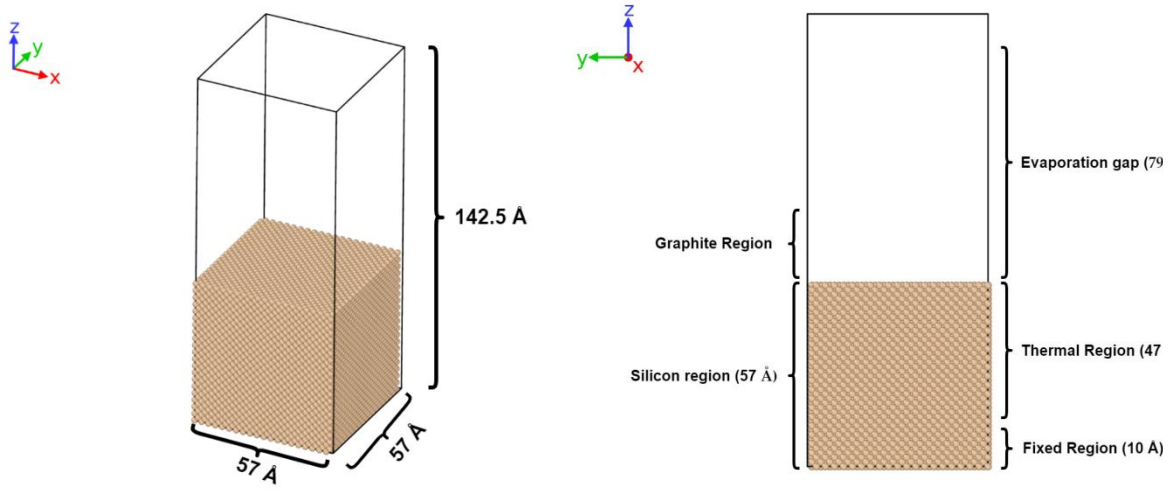


Figure 1. Dimension and region division of silicon substrate

Carbon atoms will be subjected to temperatures of 800°C, 1100°C, and 1400°C, which aligns with experimental carbon evaporation deposition research. This evaporation simulation employed the Tersoff potential function to model the interactions between silicon and carbon atoms. The interaction parameters for silicon-silicon and silicon-carbon interactions are presented in Table 1 and Table 2, respectively. As the carbon adheres to the substrate, the temperature was then gradually decreased to room temperature (300 K) and subsequently held constant by applying the canonical ensemble. In this ensemble, the number of atoms (N), volume (V), and temperature (T) are kept constant, also known as the NVT ensemble. The deposition simulation will last for 600 picoseconds, and the results will be presented by slicing the carbon atoms above the substrate by 10 angstroms using the slice feature. The number of atoms above the substrate will be analyzed using the select atom type feature from OVITO [9] after 100 picoseconds, 300 picoseconds, and 600 picoseconds.

Table 1. Tersoff parameters for Si-Si interaction[10]

A = 3264.7 eV	B = 95.373 eV	
λ_1 = 3.2394 Å−1	λ_2 = 1.3258 Å−1	n = 22.956
α = 0	β = 0.33675	h = 0.0000
c = 4.881	d = 2.0417	D = 0.2 Å
$\lambda_3 = \lambda 2$	R = 3.0 Å	

Table 2. Tersoff parameters for Si-C interaction [11]

Parameter	C	Si	Si-C
R^e (Å)	1.515	2.197	1.7631
D^e (eV)	4.265	2.887	4.682
β (Å)	1.50	1.469	1.728
S	1.44	1.32	1.541
δ	0.80469	0.78	-
R^1 (Å)	2.2	2.2	2.2
R^2 (Å)	2.5	2.5	2.5
A	0.011304	0.013318	-
c	19	14	-
d	2.5	2.1	-

RESULT AND DISCUSSION

Simulation Result

These molecular dynamics simulations revealed a progressive increase in the number of carbon atoms deposited on the silicon substrate during the 800°C treatment. At 100 picoseconds (ps), 225 carbon atoms were observed, followed by a rise to 910 atoms at 300 ps and 1025 atoms at 600 ps. These simulations were performed within a simulation box encompassing the outermost layer of silicon and the initial layer of graphite, with a layer height of 10 angstroms. Notably, the total number of carbon atoms generated within the simulation box at 100 ps, 300 ps, and 600 ps was 500, 1500, and 3000, respectively.

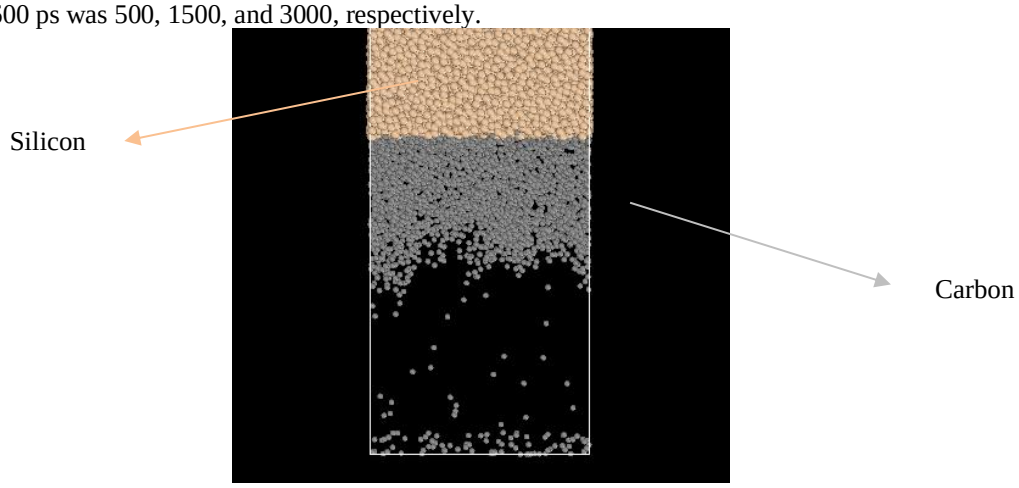


Figure 2. A snapshot of the side view illustrating the deposition of carbon atoms from graphite onto a silicon substrate under conditions of 800°C and a deposition time of 600 picoseconds

Figure 2 depicts carbon atoms as small gray spheres with darker regions, indicating uncovered portions of the substrate. The simulated layers demonstrate temporal variations in their formation. As shown in Figure 3, time significantly influences the number of deposited atoms; longer simulation times correlate with increased carbon atom deposition. However, the deposition rate is not uniform. For instance, a substantial increase from 225 atoms at 100 ps to 910 atoms at 300 ps is observed.

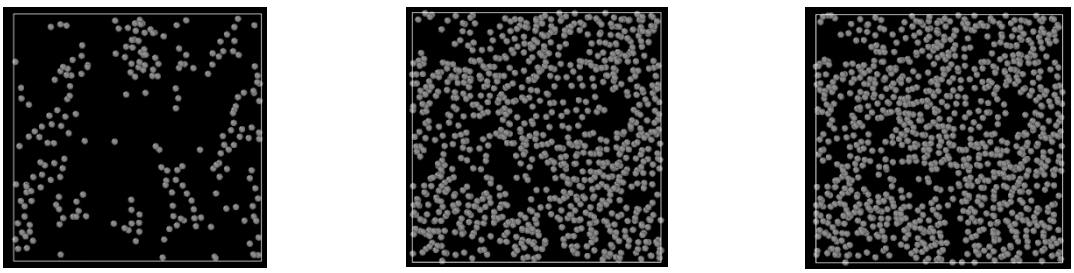


Figure 3. A snapshot of a bottom view illustrating the deposition of carbon atoms from graphite onto a silicon substrate under conditions of 800°C and deposition times of 100, 300, and 600 picoseconds.

After 600 ps, the deposition process resulted in 1025 carbon atoms being incorporated into the substrate. The increment in the number of deposited carbon atoms between 300 ps and 600 ps was only 115 atoms. These findings indicate that the carbon atoms deposited earlier obstructed, to some extent, the deposition sites for the incoming carbon atoms during this timeframe. Thus hindering the penetration of subsequent carbon atoms into the 10-angstrom layer. Consequently, 300 ps emerges as the optimal treatment time for achieving the desired 10-angstrom layer thickness, and extending the simulation beyond this point does not significantly enhance atom deposition within this layer.

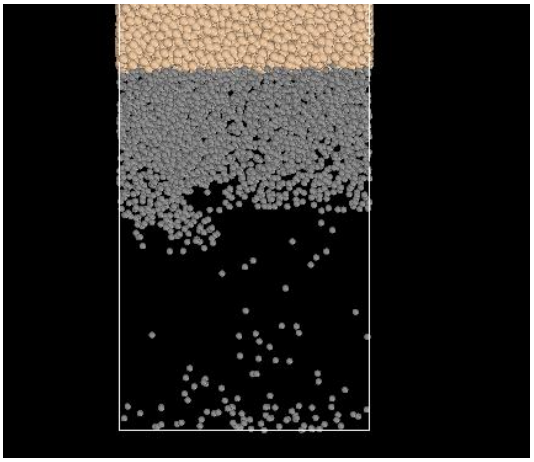
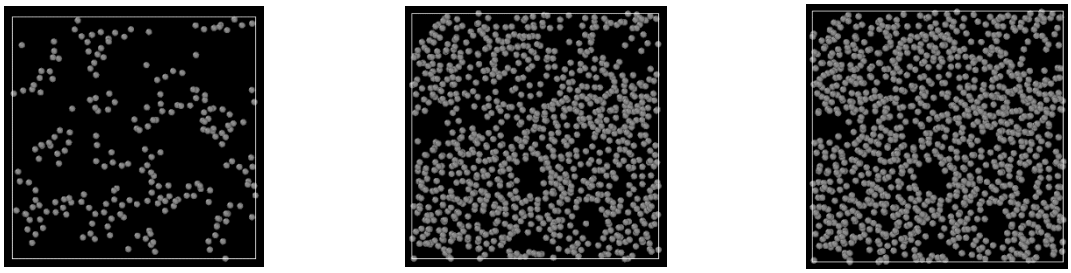


Figure 4. A snapshot of the side view illustrating the deposition of carbon atoms from graphite onto a silicon substrate under conditions of 1100°C and a deposition time of 600 picoseconds

These molecular dynamics simulations at 1100°C revealed a progressive increase in carbon atom deposition on the silicon substrate (see Figure 4)**.** After 100 ps, 246 carbon atoms were observed, followed by a rise to 1008 atoms at 300 ps and 1109 atoms at 600 ps. These atoms were localized within a 10-angstrom layer, positioned approximately 5.9 to 6.1 angstroms above the substrate. Within the simulation box, the total number of carbon atoms generated at 100 ps, 300 ps, and 600 ps was 500, 1500, and 3000, respectively.



a) b) c)

Figure 5. A snapshot of a bottom view illustrating the deposition of carbon atoms from graphite onto a silicon substrate under conditions of 1100°C and deposition times of 100, 300, and 600 picoseconds.

While the overall deposition trends were similar to those observed at 800°C, the impact of treatment duration on carbon atom deposition was particularly pronounced at 1100°C. Figure 5 shows that longer treatment times consistently led to higher deposition rates, emphasizing the importance of this variable in our study. A notable difference was the increased number of carbon atoms deposited at 10 angstroms above the substrate. The 1100°C treatment yielded a significantly higher quantity of atoms compared to the 800°C treatment.

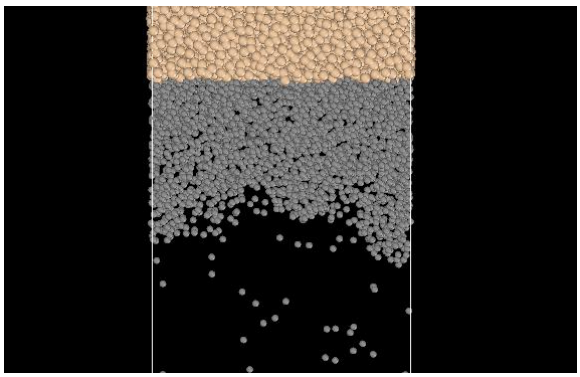


Figure 6. A snapshot of a bottom view illustrating the deposition of carbon atoms from graphite onto a silicon substrate under conditions of 1400°C and deposition times of 100, 300, and 600

These molecular dynamics simulations at 1100°C also revealed a progressive increase in carbon atom deposition on the silicon substrate**.** After 100 ps, 253 carbon atoms were observed, followed by a rise to 938 atoms at 300 ps and 1063 atoms at 600 ps. These atoms were localized within a 10-angstrom layer, positioned approximately 5.9 angstroms above the substrate. Within the simulation box, the total number of carbon atoms generated at 100 ps, 300 ps, and 600 ps was 500, 1500, and 3000, respectively.

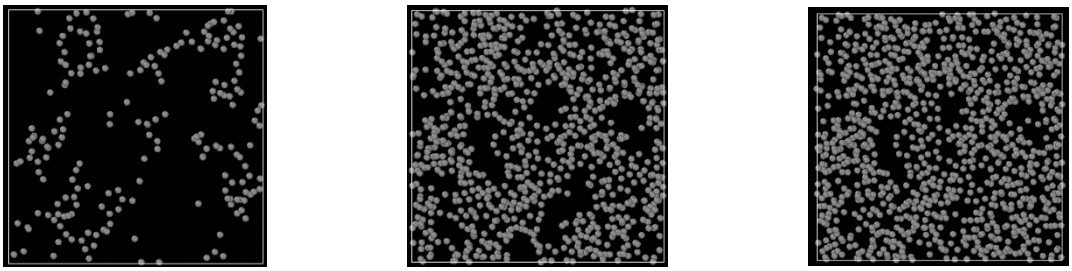


Figure 7. A snapshot of a bottom view illustrating the deposition of carbon atoms from graphite onto a silicon substrate under conditions of 1400°C and deposition times of 100, 300, and 600 picoseconds.

While the overall deposition trends were similar to those observed at lower temperatures, as depicted by Figure 6 and Figure 7, the 1400°C treatment exhibited a notable difference**.** Although a clear correlation between treatment duration and carbon atom deposition was maintained, the maximum number of atoms deposited at the substrate distance did not exceed that achieved at 1100°C. This discrepancy might be attributed to the increased kinetic energy of carbon atoms at higher temperatures, leading to a higher probability of them rebounding from the substrate surface rather than adhering to it. The simulated carbon layer exhibited the characteristic features of an amorphous structure. Thin films fabricated via physical vapor deposition (PVD) commonly exhibit an amorphous structure [12].

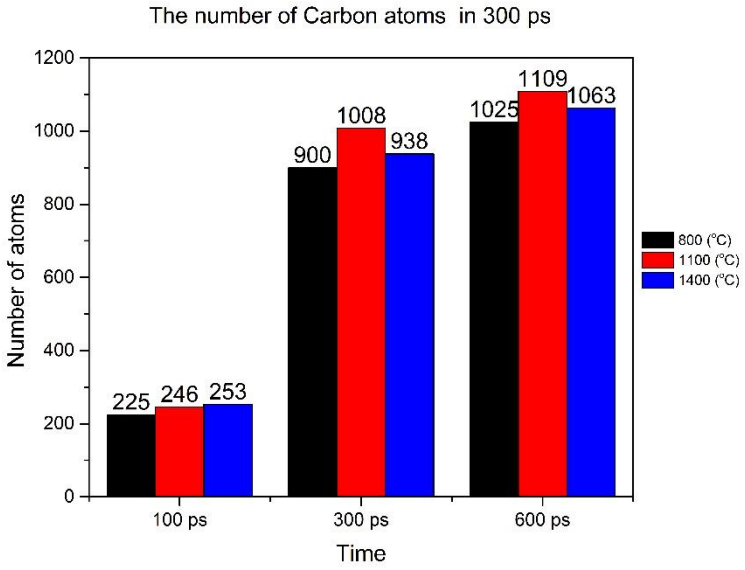


Figure 8. Carbon atom density on a silicon substrate as a function of temperature in 300 ps

Figure 8 shows that the quantity of atoms adhering to and penetrating the substrate increases linearly with temperature after 300 ps of deposition. As the temperature rises, the depth of atomic penetration into the substrate also increases. Nevertheless, beyond 600 ps, the rate of atomic absorption by the substrate significantly diminishes. This phenomenon can be explained by the formation of a dense surface layer that acts as a barrier to further atomic diffusion. Moreover, the quantity of atoms absorbed at 1400°C is lower compared to 100°C, suggesting that a portion of the carbon atoms at such elevated temperatures are desorbed from the substrate.

Radial Distribution Function

Consistent with the preceding discussion on carbon deposition, the radial distribution function (RDF) results (Figure 9) within a 300 ps timeframe indicate that the RDF intensity of carbon at 1100K is maximal, surpassing that at 1400K. This finding reinforces the suggestion that a 300 ps duration is insufficient for a significant portion of carbon atoms to complete diffusion and to distribute uniformly within the substrate. The optimal temperature is 1100K, whereas, at 1400 K, it is plausible that some carbon atoms with higher kinetic energy lack sufficient time to find stable positions within the substrate and may instead rebound from the substrate surface.

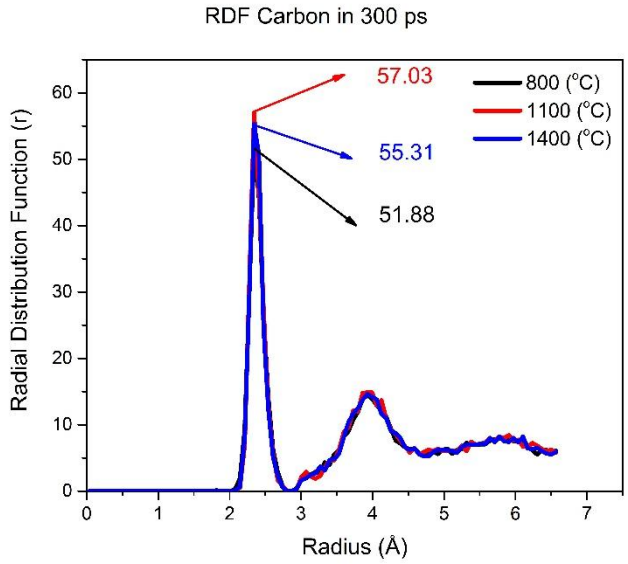


Figure 9. The radial distribution functions of carbon atoms at temperatures of 800°C, 1100°C, and 1400 °C over a simulation period of 300 picoseconds

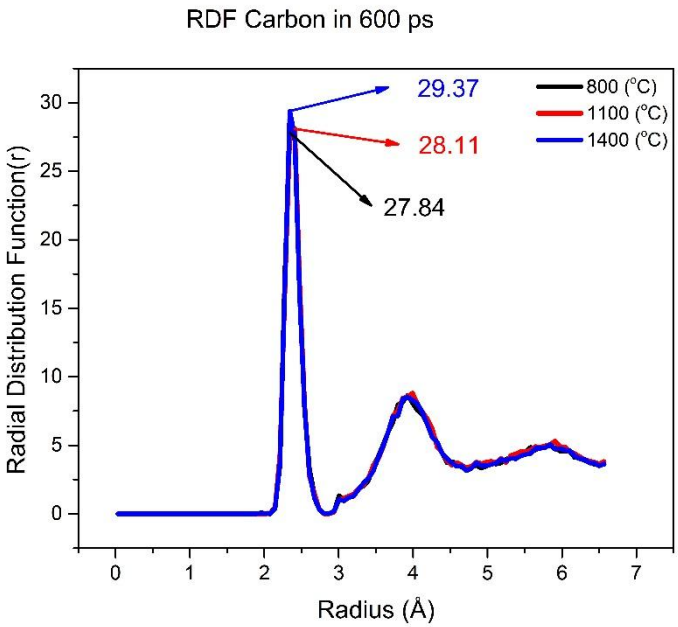


Figure 10. The radial distribution functions of carbon atoms at temperatures of 800°C, 1100°C, and 1400°C over a simulation period of 600 picoseconds

Figure 10 shows distinct RDF results observed for a 600 ps timeframe. The RDF intensity increases with increasing temperature, reaching a maximum at 1400 K. This indicates that carbon atoms have ample time to locate stable positions within the substrate and distribute more uniformly. The increased number of nearest neighbors at a specific distance results in a higher peak in the RDF intensity.

CONCLUSION

These molecular dynamics simulations have revealed a complex interplay between temperature and deposition time in influencing the quantity and distribution of deposited carbon atoms on a silicon substrate. Within a 300 ps deposition timeframe, the relationship between temperature and carbon deposition is non-linear. This suggests that the 300 ps duration is insufficient for carbon atoms to fully diffuse and distribute uniformly, leading to the accumulation of carbon atoms at higher temperatures (1400K) due to hindered diffusion of subsequent atoms. In contrast, a 600 ps deposition period exhibits a clear positive correlation between temperature and carbon deposition. The extended duration allows carbon atoms to disperse more evenly, creating vacancies for additional carbon atoms to occupy within the substrate. This enhanced mobility at higher temperatures promotes more uniform carbon distribution and increases the overall deposition rate.

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