

Molecular Dynamics Simulations of Surface Melting in FCC, BCC, and HCP Metals: Influence

of Surface Orientation and System Size on Melting Temperature and Diffusion Properties

Anna Tretiakova U85699463

ME 306 Extra Credit Assignment

Introduction

Molecular dynamics (MD) simulations have become a powerful tool for studying atomic-scale phenomena such as melting, surface dynamics, and diffusion in metals. By numerically integrating Newton's equations of motion, MD enables researchers to model the time evolution of atomistic systems with high spatial and temporal resolution [7]. One of the phenomena that MD can uniquely capture is the transition between solid and liquid phases in metals. These effects show up differently on different atomic arrangements and different crystallographic planes. The most common crystal structures in metals include simple cubic (SC), face centered cubic (FCC), body centred cubic (BCC), and hexagonal close packed (HCP) [5]. For this report, three metals with different crystal structures were selected: aluminum with an FCC structure, tungsten with a BCC structure and titanium with an HCP structure. Figure 1.1 illustrates the FCC, BCC, and HCP unit cells, along with a red representation of the planes examined. For the cubic unit cells, the [100], [110], and [111] planes were considered, while for the HCP system, the corresponding basal [0001], prismatic [1100], and pyramidal [0111] planes were analyzed. The HCP system uses a four-axis coordinate system, which is why different planes were required.

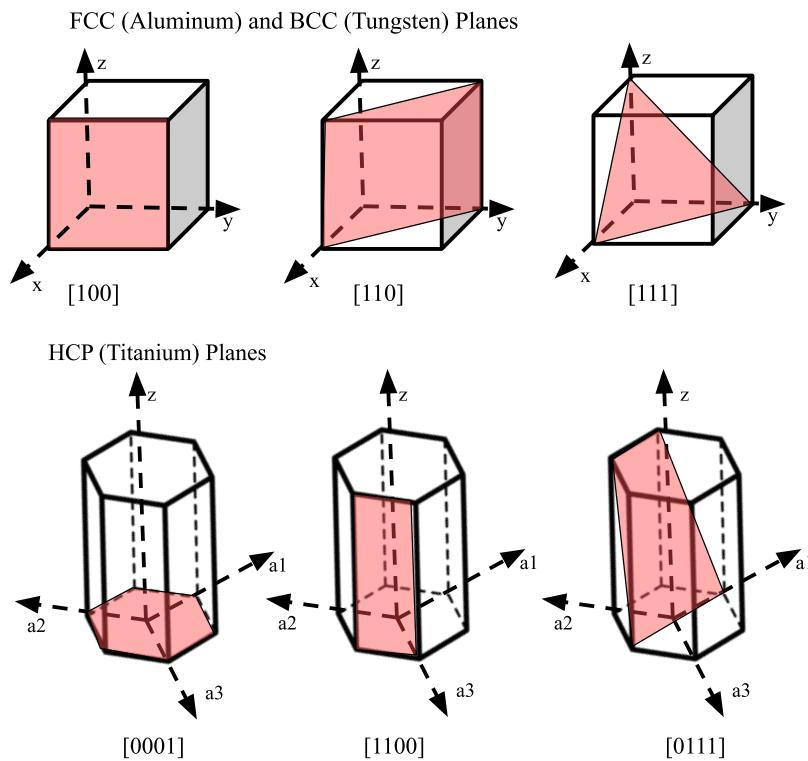


Figure 1.1: The Planes Examined in the Metals with FCC, BCC and HCP Crystal Structures

Even though this report will refer to the transition between solid to liquid as melting temperature, the simulation is not actually melting the metal, instead it is super heating it. Melting is when the metal is slowly heated until it reaches the melting temperature, which is the point where this metal exists at equilibrium between the solid and liquid phases [6]. Superheating on the other hand is when the metal is heated quickly to a temperature above its melting point [8] and the temperature at which the atomic mean square displacement (MSD) transitions from linearly increasing to exponentially increasing is taken to be the melting point. Since each plane's structure exhibits unique surface energetics and diffusion pathways that influence how and when melting occurs, this report will be more focused on comparing the different crystallographic planes' behaviours in superheating conditions, other than determining the accurate melting point. From the plotted MSD vs time of each surface, the diffusivity constant can be calculated from finding the slope of the linear parts. The diffusivity constant is a measure of how quickly atoms or molecules spread through a material over time due to thermal motion, which is influenced by the atomic structure and bonding of the material, the presence of defects or impurities, and the specific crystallographic direction in anisotropic materials [4]. The surface energy of each plane can be calculated with equation 1 and plotted vs time:

$$\gamma = \frac{E_{\text{slab}} - N * E_{\text{bulk}}}{2A} \quad (1)$$

Where γ is the surface energy, E_{slab} is the total energy of the plane surface, N is the number of atoms on the plane surface, E_{bulk} is the energy per atom in the entire bulk material, A is the surface area of planes surface and the factor of 2 accounts for the fact that there are two sides to each plane surface [9]. In addition, the kinetic energy, maximum force and radial distribution function (RDF) for each of the metals will be examined to gain insight into their melting behavior. Kinetic energy over time is directly related to the system's temperature and helps show the rate at which the system was heated. Maximum force over time reveals moments when atoms experience intense interactions, which can indicate mechanical instability or the beginning of a structural breakdown. The RDF reflects how the density of atoms varies as a function of distance from a reference atom [4]. Together, these metrics offer a comprehensive view of the dynamic processes occurring during heating of the three different metals.

Methods

Before making or running any simulations, the interatomic potentials for the metals aluminum, tungsten and titanium were found through the NIST Interatomic Potential Repository. Aluminum is an FCC metal [1], tungsten is a BCC metal [2] and titanium is an HCP metal [3]. The LAMMPS software was used to run all of the simulations. The input code was written in Visual Studio Code and then ran in the command prompt of a Windows 10 computer. All data analysis and plots were done in MATLAB R2024a and the atoms were visualized in OVITO - Open Visualization Tool. ChatGPT [10] was used to help debug the LAMMPS and MATLAB code. To ensure reliable results in this study, a systematic, step-by-step approach was implemented to determine the appropriate number of atoms required for each simulation. In

order to create atoms in a LAMMPS simulation, a region must first be defined, typically as a cube or rectangular prism where atoms are placed according to the chosen lattice and orientation. Multiple cube sizes were tested to evaluate how simulation results varied with system size, particularly in terms of the MSD of the total system over time. Very small cubes did not show a clear transition from the linear change in MSD to exponential change in MSD. After comparing different configurations for all metals, a $7 \times 7 \times 7$ lattice was found to be the most effective. It was large enough to minimize surface and finite-size effects, while still being computationally efficient. This size struck an ideal balance between accuracy and performance, ensuring that the simulation results were both reliable and manageable in terms of simulation time. Figure A.1 presents the measured physical dimensions of the simulation region for each metal when defining a $7 \times 7 \times 7$ lattice unit region in LAMMPS using metal-specific interatomic potentials. These perfect cubes of each metal were used to make the kinetic energy, maximum force, MSD over time and RDF plots. To evaluate surface-specific properties, each simulation cube was oriented according to the target crystallographic plane. Beginning with a single atomic layer, simulations were conducted to plot the MSD vs temperature and surface energy, as well as to calculate the diffusion constant for each plane surface. This process was repeated with up to 8 atomic layers for each plane in each metal. These can be seen in Appendix section B for aluminum, section C for tungsten and section D for titanium. Each section has 8 tables, and each table has an OVITO screenshot of the plane, the number of atoms, the mentioned plots and calculated values. Based on the analysis of all plots, the optimal number of atoms for accurate and reliable simulation results was identified. The rationale and detailed explanation for the selected number of atoms for each metal are provided in the Results section.

Results

The kinetic energy vs. time plots offer a clear visualization of how atomic motion evolves during heating [4]. Since temperature is directly proportional to the average kinetic energy of atoms, a linear increase in kinetic energy over time is expected in a controlled heating simulation. In this study, using $7 \times 7 \times 7$ lattice cubes, the kinetic energy increased steadily with time, confirming that the systems were heating uniformly. Figures 2.11, 2.12, and 2.13 show the kinetic energy versus time for aluminum, tungsten, and titanium, respectively. All metals start off at room temperature and are heated beyond their melting points: 933K for aluminum, 3673K for tungsten and 1943K for titanium [6]. All systems exhibit similar starting and ending kinetic energies because, despite having different melting temperatures, each was heated the same amount beyond its respective melting point.

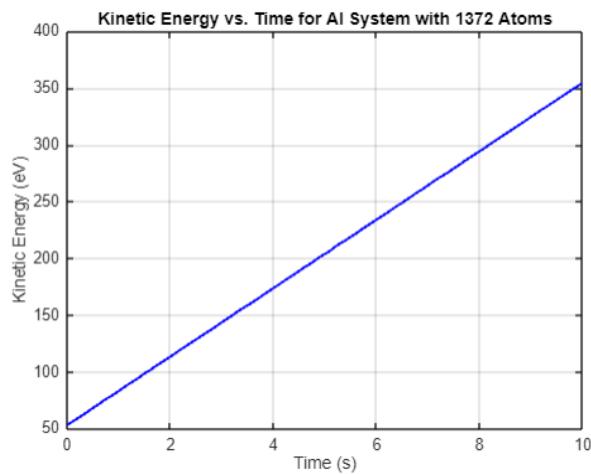


Figure 2.11: Kinetic Energy vs Time For Al System

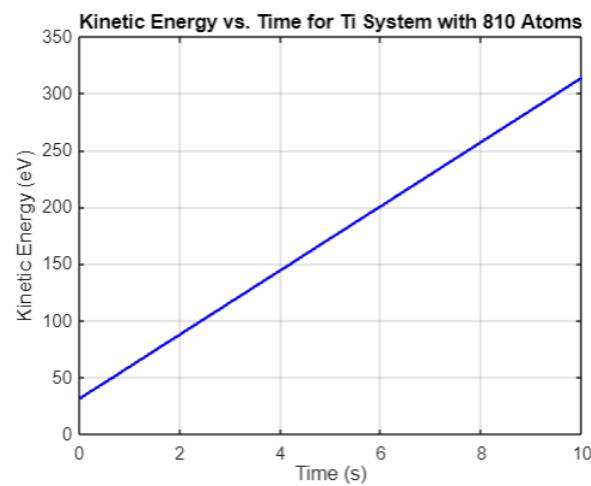


Figure 2.12: Kinetic Energy vs Time For W System

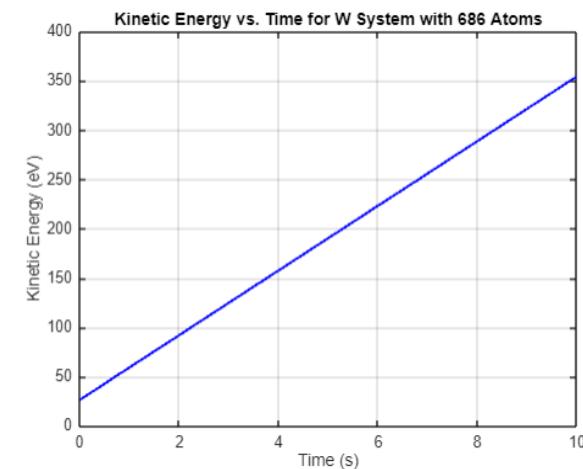


Figure 2.13: Kinetic Energy vs Time For Ti System

The maximum force vs. time plots track the maximum force experienced by any atom in the simulation over time. This metric helps assess system stability and structural integrity during heating or other simulation processes. Sudden spikes in the maximum force can indicate atomic rearrangements, such as melting, defect formation, or surface reconstruction [4]. Figures 2.21, 2.22 and 2.23 show the maximum force vs time for aluminum, tungsten, and titanium, respectively. For all metals, the initial fluctuations in maximum force were minimal, but increased significantly as the temperature rose and the materials approached the liquid phase.

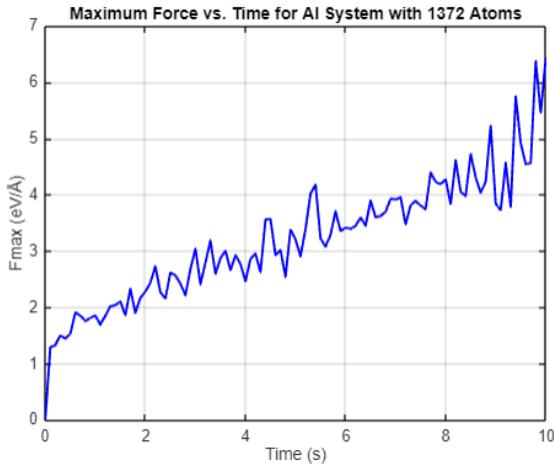


Figure 2.21: Maximum Force vs Time For Al System

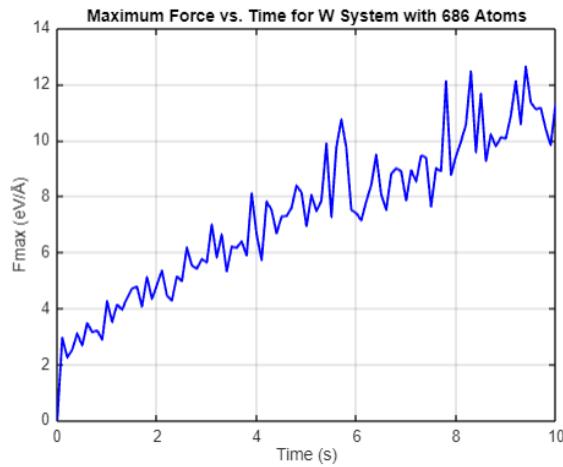


Figure 2.22: Maximum Force vs Time For W System

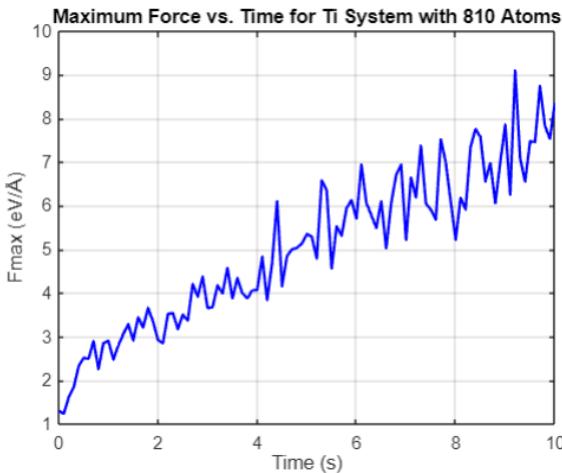


Figure 2.23: Maximum Force vs Time For Ti System

The MSD vs. time plots illustrate how atomic motion evolves during the simulation. At lower temperatures, atoms vibrate around their equilibrium positions, resulting in relatively flat or linear MSD curves. As temperature increases and the system nears or surpasses the melting point, atoms begin to diffuse more freely, causing the MSD to rise more sharply, indicating a transition from solid-like to liquid-like behavior. This pattern helps identify melting behavior and assess atomic mobility across different conditions. Figures 2.31, 2.32, and 2.33 show the MSD vs. time for aluminum, tungsten, and titanium, respectively.

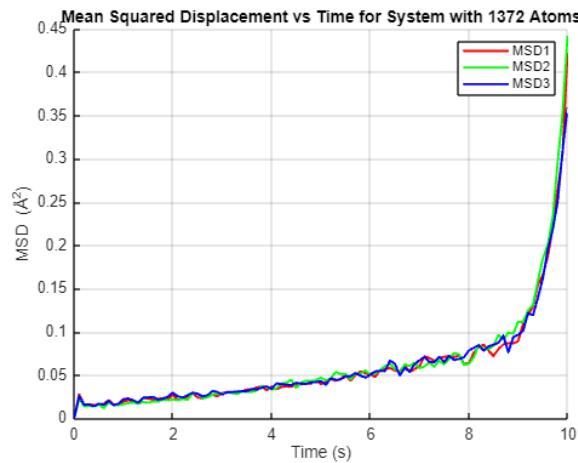


Figure 2.31: Atomic Mean Square Displacement (MSD) vs. Time For Al System

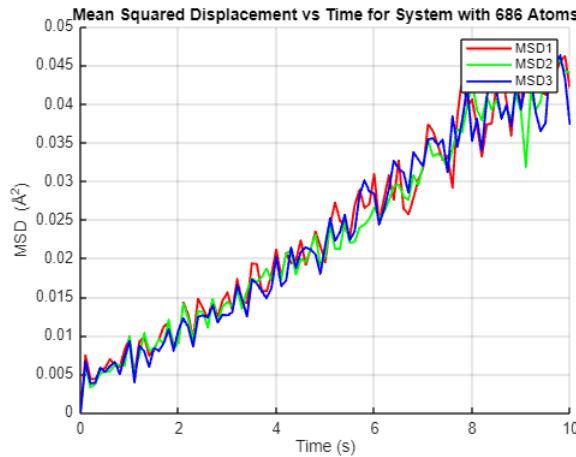


Figure 2.32: Atomic Mean Square Displacement (MSD) vs Time For W System

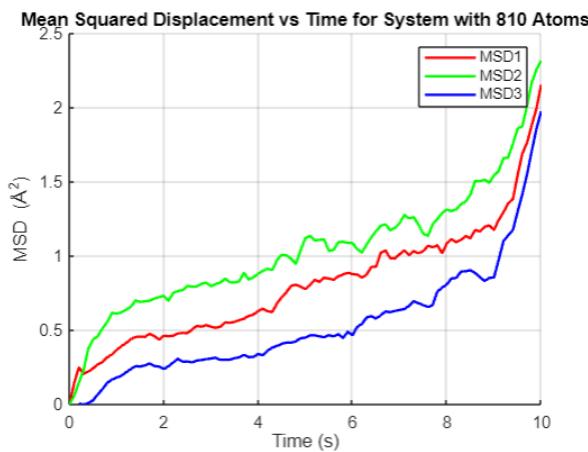


Figure 2.33: Atomic Mean Square Displacement (MSD) vs Time For Ti System

The RDF shows how atoms are spatially arranged around a reference atom. Figures 2.41, 2.42, and 2.43 show the RDF plots for aluminum, tungsten, and titanium, respectively. In tungsten, the RDF plot is cut off at a distance of 4.3 Å due to a "ghost atom" issue in the LAMMPS simulation. This occurs when atoms, particularly at the surface, are duplicated or improperly calculated, leading to spurious peaks beyond the expected atomic structure. These ghost atoms artificially extend the RDF, causing the data to abruptly end at 4.3 Å, where the system's true atomic structure is disrupted by this computational artifact.

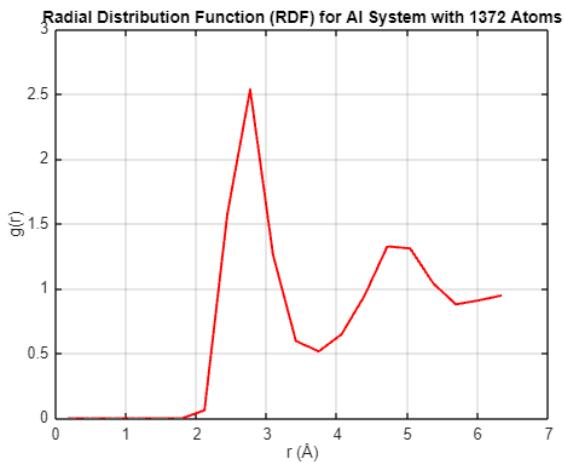


Figure 2.41: Radial Distribution Function Changes For Al System

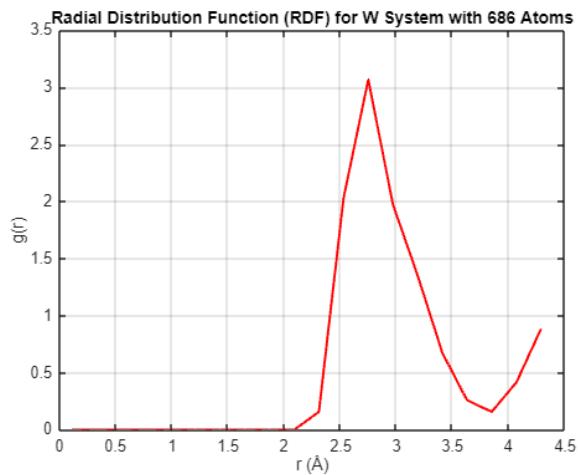


Figure 2.42: Radial Distribution Function Changes For W System

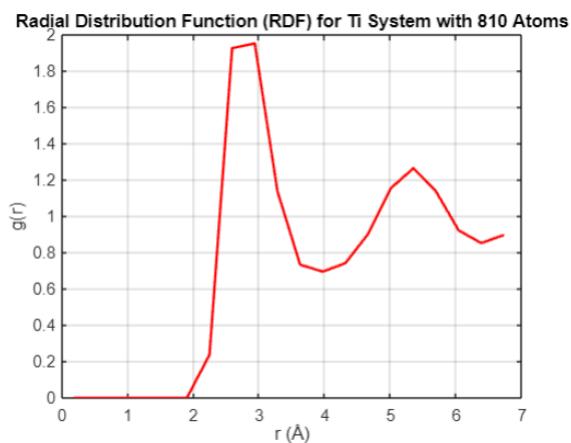


Figure 2.43: Radial Distribution Function Changes For Ti System

From Section B in the appendix, it was determined that the ideal number of atoms for this report for aluminum is about 1200 for each plane. Table 1.1 shows the results for each plane, including the exact number of atoms on the plane, the calculated melting temperature and the diffusivity constant. Figure B.6 shows that at this amount of atoms, the MSD vs temperature graphs are very cohesive and clearly show the transition between linear behaviour and exponential behaviour. The 111 plane of the aluminum does have a bigger melting temperature due to the atoms being more packed on this plane. The behaviour and result of the 100 and 110 planes are very similar, because the atoms on the planes are packed in the same way. Figures 3.11, 3.12, and 3.13 show the plotted surface energy vs. time for the 100, 110, and 111 planes respectively. Once again, the surface energy for 100 and 110 planes are very similar and the surface energy for the 111 plane is a little bigger due to the atoms being more packed.

Aluminum	Plane [100]	Plane [110]	Plane [111]
Ideal Number of Atoms	1176	1200	1247
Melting Temperature (K)	1286	1290	1439
Diffusivity Constant ($\text{\AA}/\text{s}$)	$2.616\text{e+}07 \text{\AA}^2/\text{s}$	$2.564\text{e+}07 \text{\AA}^2/\text{s}$	$2.296\text{e+}08 \text{\AA}^2/\text{s}$

Table: 1.1: The Chosen Ideal Number of Atoms for Aluminum Planes and the Corresponding Melting Temperatures and Diffusivity Constants

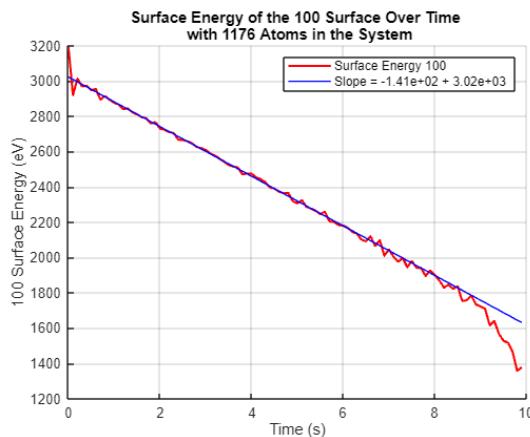


Figure 3.11: Surface Energy vs Time for Al 100 Plane

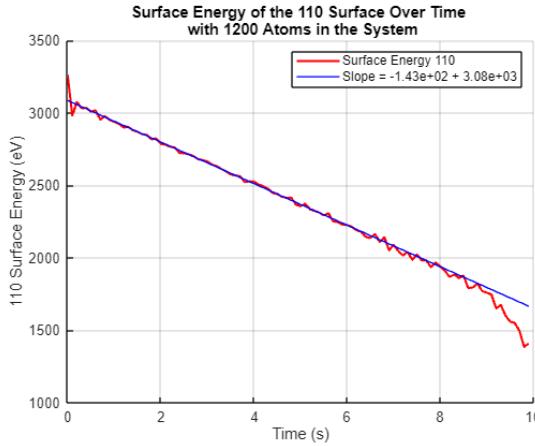


Figure 3.12: Surface Energy vs Time for Al 110 Plane

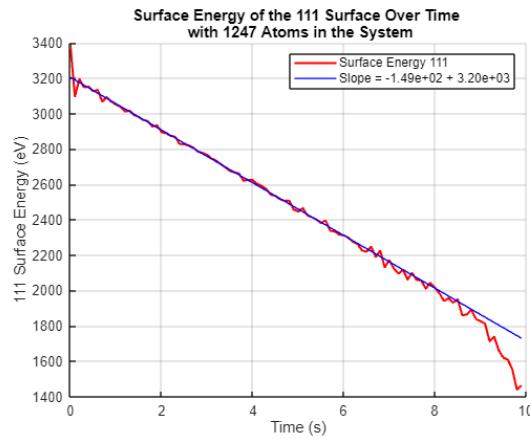


Figure 3.13: Surface Energy vs Time for Al 111 Plane

From Section C in the appendix, it was determined that the ideal number of atoms for this report for Tungsten is about 600 for each plane. Table 1.2 shows the results for each plane, including the exact number of atoms on the plane, the calculated melting temperature and the diffusivity constant. Figure C.6 shows that at this amount of atoms, the MSD vs temperature graphs have the most clear transition between linear behaviour and exponential behaviour. Even though the melting temperature is about the same for all the planes, the diffusivity constant for plane 111 is significantly greater. This is because the atoms at that plane are very spaced out, yet still have strong bonds between each other. This means that atoms have an easier time moving through this plane [4]. Figures 3.21, 3.22 and 3.23 show the plotted surface energy vs time for the planes 100, 110, and 111 respectively. The surface energy for planes 100 and 110 is about the same, while the surface energy for plane 111 is significantly greater than the rest. This increased surface energy on the plane 111 is also reflected in the diffusivity constant of the plane. This is because the 111 plane in tungsten has a higher atomic packing density, leading to greater surface energy and increased atomic mobility, which raises the diffusivity constant.

Tungsten	Plane [100]	Plane [110]	Plane [111]
Ideal Number of Atoms	588	600	619
Melting Temperature (K)	3306	3378	3556
Diffusivity Constant ($\text{\AA}/\text{s}$)	$3.134\text{e+}06 \text{\AA}^2/\text{s}$	$3.399\text{e+}06 \text{\AA}^2/\text{s}$	$7.211\text{e+}08 \text{\AA}^2/\text{s}$

Table: 1.2: The Chosen Ideal Number of Atoms for Tungsten Planes and the Corresponding Melting Temperatures and Diffusivity Constants

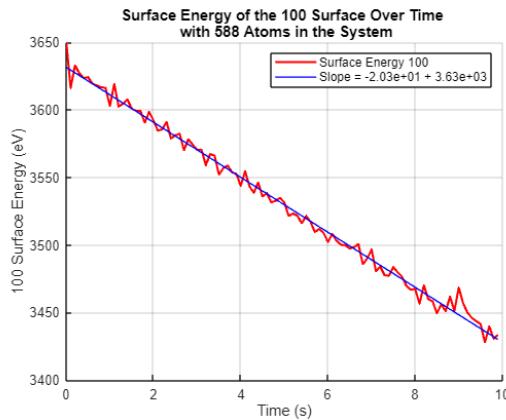


Figure 3.21: Surface Energy vs. Time for W 100 Plane

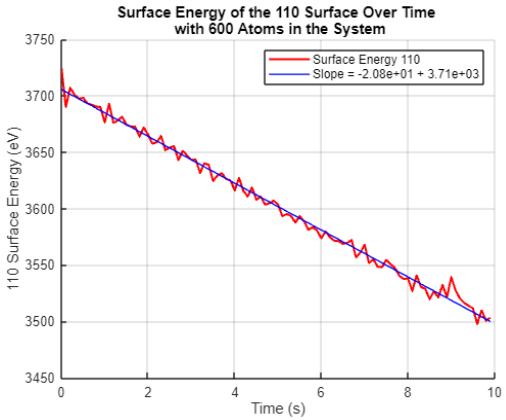


Figure 3.22: Surface Energy vs. Time for W 110 Plane

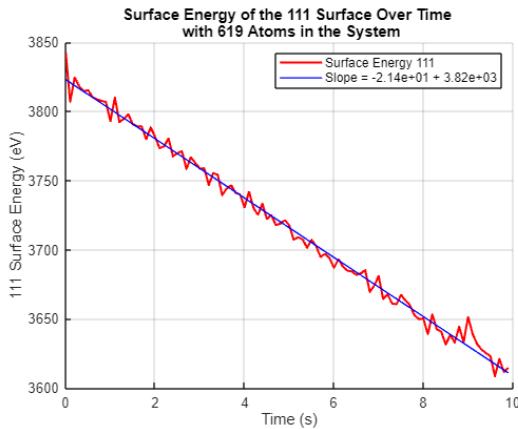


Figure 3.23: Surface Energy vs. Time for W 111 Plane

From Section D in the appendix, it was determined that the ideal number of atoms for this report for titanium is about 960 for each plane. Table 1.3 shows the results for each plane, including the exact number of atoms on the plane, the calculated melting temperature and the diffusivity constant. Figure D.6 shows that at this amount of atoms, the MSD vs. temperature graphs stay the same as more atoms are added to the simulation system. In this metal, the 0001 plane has the highest melting temperature, due to the most packed atoms. Figures 3.31, 3.32, and 3.33 show the plotted surface energy vs. time for the planes 0001, 1100 and 0111 respectively. The results were unexpected: the 0001 plane exhibited the highest surface energy, followed closely by the 1100 plane, while the 0111 plane had a surface energy an order of magnitude lower. This unexpected result may be due to anisotropic bonding in HCP structures, where the 0111 plane exposes fewer broken bonds or more stable atomic configurations, leading to significantly lower surface energy compared to the densely packed but less energetically favorable 0001 and 1100 planes.

Titanium	Plane [0001]	Plane [1100]	Plane [0111]
Ideal Number of Atoms	972	960	962
Melting Temperature (K)	1783	1568	1495
Diffusivity Constant ($\text{\AA}/\text{s}$)	$2.767\text{e+}08 \text{\AA}^2/\text{s}$	$3.212\text{e+}08 \text{\AA}^2/\text{s}$	$4.904\text{e+}08 \text{\AA}^2/\text{s}$

Table: 1.3: The Chosen Ideal Number of Atoms for Titanium Planes and the Corresponding Melting Temperatures and Diffusivity Constants

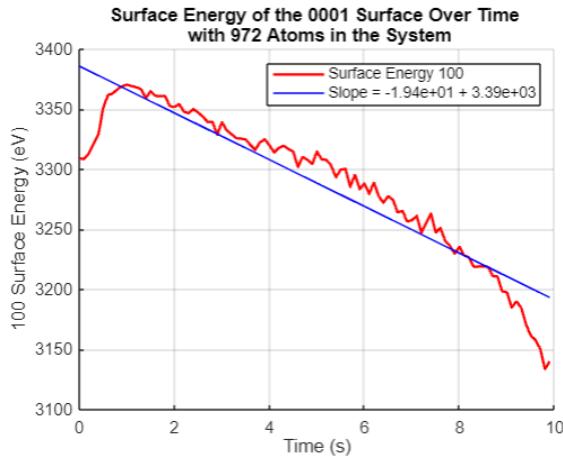


Figure 3.31: Surface Energy vs. Time for Ti 0001 Plane

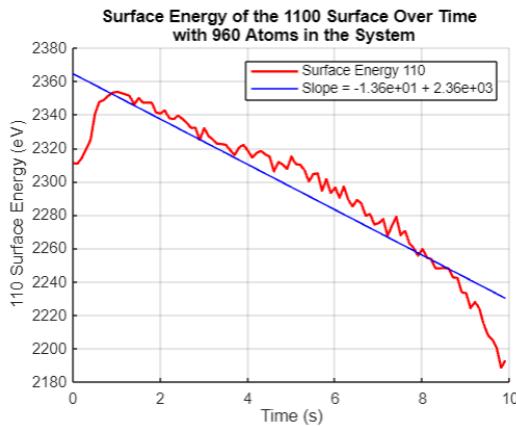


Figure 3.32: Surface Energy vs. Time for Ti 1100 Plane

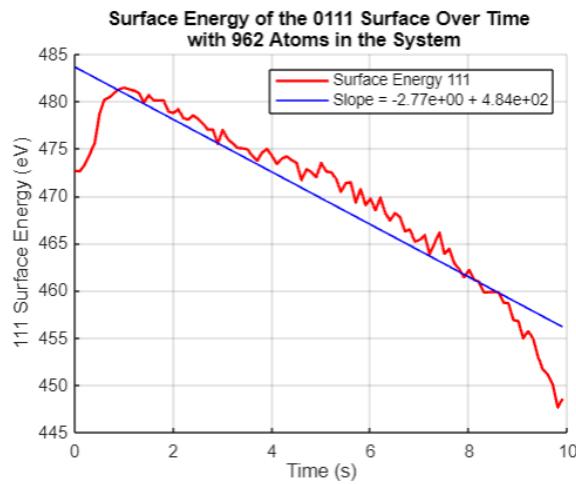


Figure 3.33: Surface Energy vs. Time for Ti 0111 Plane

For all metals and planes, the surface energy decreased linearly with increasing temperature due to the decrease in the surface tension [11]. In this report the results were, as

temperature increases, atomic bonds weaken and atoms move farther apart, reducing the surface energy of the plane.

Discussion

The surface plane had a significant influence on the observed melting temperature due to variations in atomic packing density and coordination number at different crystallographic orientations. Densely packed planes, such as the 111 plane in FCC metals, generally exhibited higher melting temperatures compared to less densely packed planes like 100 or 110. This is because atoms on tightly packed surfaces are more strongly bound, requiring more thermal energy to overcome cohesive forces and initiate melting [6]. In contrast, more open planes with fewer neighboring atoms per surface atom had weaker bonding and melted at lower temperatures, demonstrating the impact of atomic arrangement on thermal stability.

The number of atoms in the slab directly affects the accuracy and stability of the simulated melting temperature, especially in the systems with few atoms. Smaller systems are more susceptible to finite-size effects, such as enhanced surface-to-volume ratio and artificial stabilization or destabilization of phases, which can lead to inaccurate melting behavior. Increasing the number of atoms improves statistical sampling and better approximates bulk behavior, minimizing edge effects and allowing the system to more realistically reflect the thermodynamic properties of the material. This is very clearly demonstrated in tables B.1, B.2 and B.3. The three layer system in table B.3 has a clearer change from linear to exponential behavior in the MSD vs. temperature graphs than in the single layer system in table B.1. Thus, larger slabs tend to yield more reliable and consistent melting temperatures, up to a point where further increases result in diminishing returns and require excessively long simulation run time.

Through the completion of this MD analysis, the possibility that different interatomic potentials for the same element can yield noticeably different results is evident. All of the measured properties are sensitive to atomic interactions, such as melting temperature, diffusion coefficients, and surface energy. Each potential is parameterized based on specific datasets and fitting strategies, which may prioritize certain physical properties over others. As a result, one potential might more accurately capture elastic properties, while another may better represent phase transitions or defect behavior. Therefore, the choice of interatomic potential must align with the specific simulation goals to ensure the reliability of the predicted properties.

Several limitations in the simulation setup may have impacted the calculated properties. These include the use of finite-sized slabs, fixed boundary conditions, and assumptions inherent to classical molecular dynamics, such as neglecting quantum effects. Additionally, limitations in the precision of interatomic potentials and computational constraints restricted the number of atoms and simulation time steps, potentially influencing the accuracy of phase transition observations and kinetic measurements. These factors could lead to slight deviations in melting temperature and diffusion behavior compared to experimental data, emphasizing the need for careful calibration and validation against known benchmarks. Given more time, the same process illustrated in appendix sections B, C and D would be done for different sizes of metal blocks.

References

- [1] Sheng, H. W. (2010, May 11). *EAM potentials: Aluminum (FCC)*. Retrieved from <https://sites.google.com/site/eampotentials/al>
- [2] Mason, D. R., Nguyen-Manh, D., & Becquart, C. S. (2017). An empirical potential for simulating vacancy clusters in tungsten. *Journal of Physics: Condensed Matter*, 29(50), 505501. <https://doi.org/10.1088/1361-648X/aa9776> Retrieved from: https://openkim.org/id/Sim_LAMMPS_MEAM_Lenosky_2017_W_SM_631352869360_00
- [3] Mendelev, M. I., Underwood, T. L., & Ackland, G. J. (2016). Development of an interatomic potential for the simulation of defects, plasticity, and phase transformations in titanium. *The Journal of Chemical Physics*, 145(15), 154102. <https://doi.org/10.1063/1.4965821> Retrieved from: <https://pubs.aip.org/aip/jcp/article/145/15/154102/935538/>
- [4] Chapman, J. (n.d.). *ME306: Class notes and in-person conversations*. Department of Mechanical Engineering, Division of Materials Science and Engineering, Boston University.
- [5] National Institute of Standards and Technology (NIST). (n.d.). *NIST interatomic potential repository project*. Retrieved April 29, 2025, from <https://www.ctcms.nist.gov/potentials/>
- [6] Metal Supermarkets. (2020, June 16). *The melting points of metals*. Retrieved from: <https://www.metalsupermarkets.com/melting-points-of-metals/>
- [7] Plimpton, S., Thompson, A., & LAMMPS Developers. (2025, April 2). *LAMMPS documentation* (Version 2 Apr 2025). Sandia National Laboratories. <https://docs.lammps.org>
- [8] School of Physics, UNSW. (n.d.). Superheating and microwave ovens. Physclips. The Australian Office for Learning and Teaching. Retrieved from: <https://www.animations.physics.unsw.edu.au/jw/superheating.htm#:~:text=In%20this%20context%20superheating%20means,a%20substantial%20quantity%20of%20vapour>.
- [9] Choudhary, K., & Garrity, K. F. (2024). InterMat: Accelerating band offset prediction in semiconductor interfaces with DFT and deep learning. *Digital Discovery*, 3, 1365–1377. Retrieved from: <https://doi.org/10.1039/D4DD00031E>
- [10] OpenAI. (2025). ChatGPT (April 2025) [Large language model] <https://chat.openai.com>
- [11] Aqra, F., & Ayyad, A. (2011). Surface energies of metals in both liquid and solid states. *Applied Surface Science*, 257(17), 7446–7450. <https://doi.org/10.1016/j.apsusc.2011.01.123>

Appendix

Section A: Testing For Experimental Design

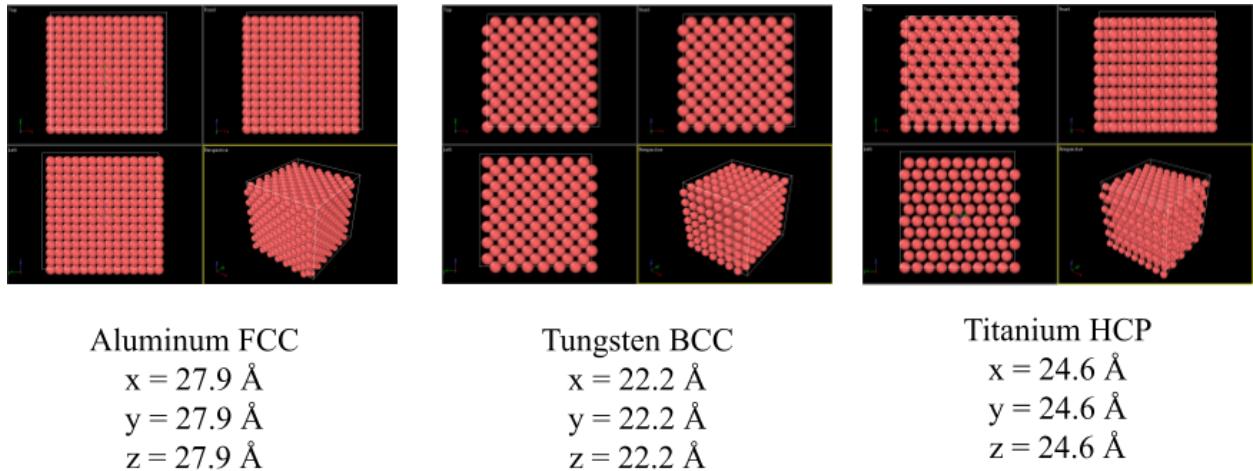


Figure A.1: Measured Dimensions of Each Metal When Defining a $7 \times 7 \times 7$ Simulation Region in LAMMPS with Metal-Specific Interatomic Potentials

Section B: Testing for The Correct Amount of Atoms For Aluminum

Table B.1: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=3.98)

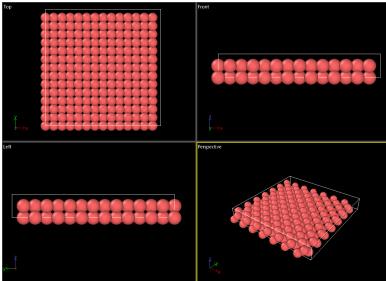
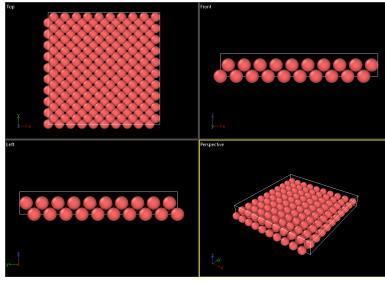
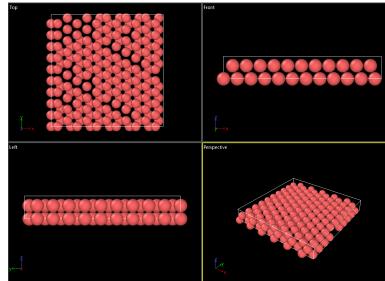
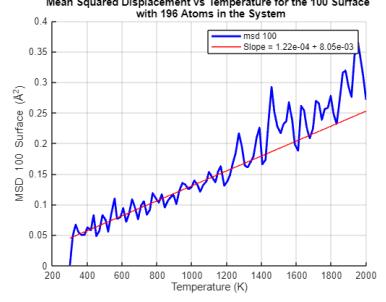
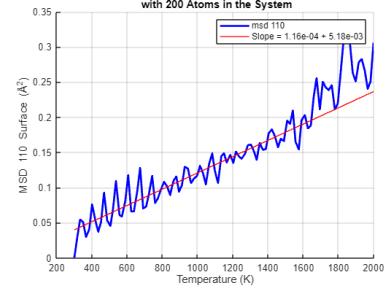
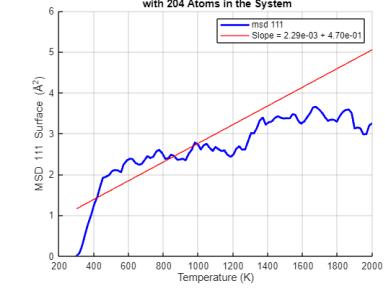
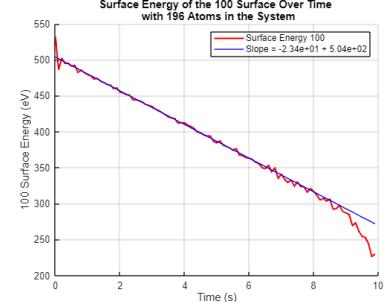
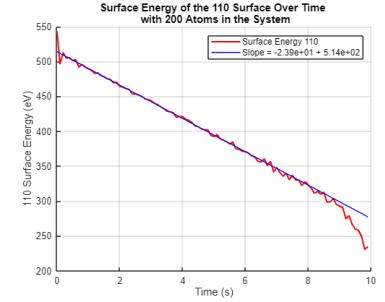
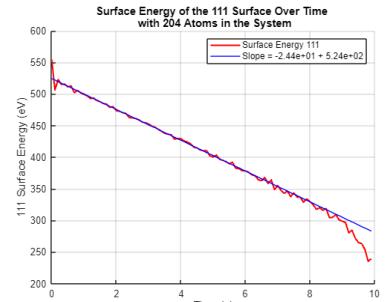
100 Plane of Al	110 Plane of Al	111 Plane of Al
 196 atoms	 200 atoms	 204 atoms
		
Temperature: 1116	Temperature: 1047	Temperature: 1218
Diffusion Constant: $3.058\text{e+}07 \text{ \AA}^2/\text{s}$	Diffusion Constant: $2.892\text{e+}07 \text{ \AA}^2/\text{s}$	Diffusion Constant: $8.163\text{e+}08 \text{ \AA}^2/\text{s}$
		

Table B.2: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=7.96)

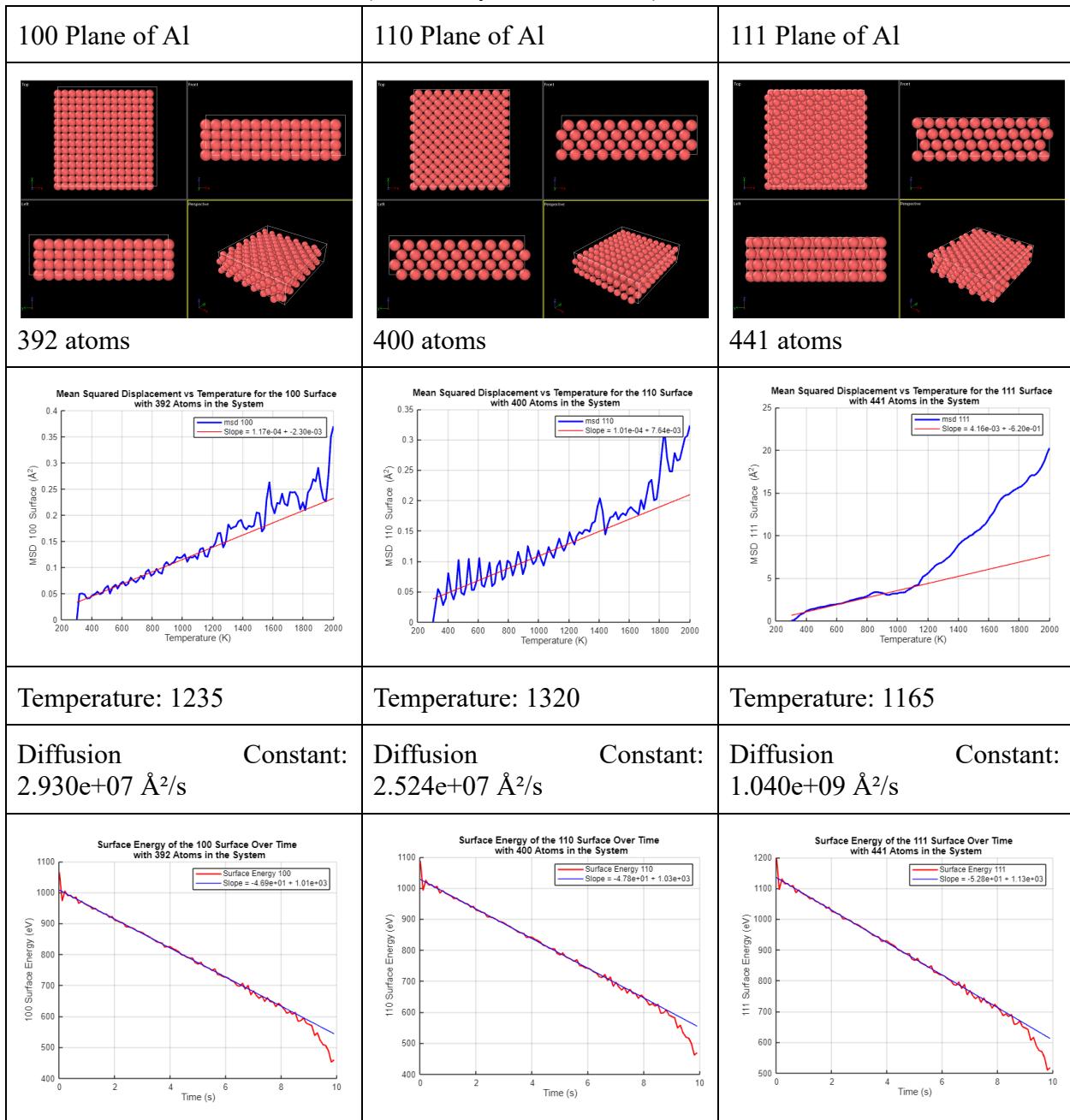


Table B.3: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=11.94)

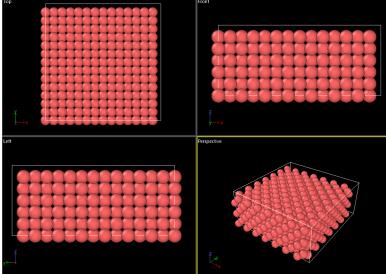
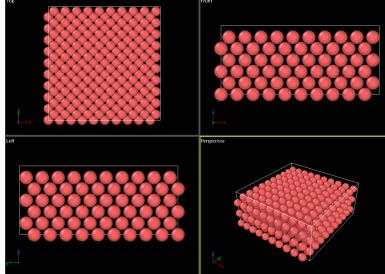
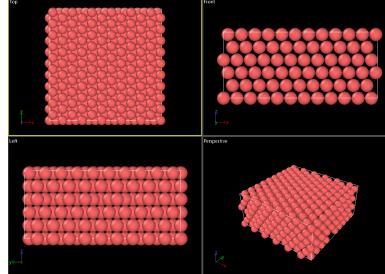
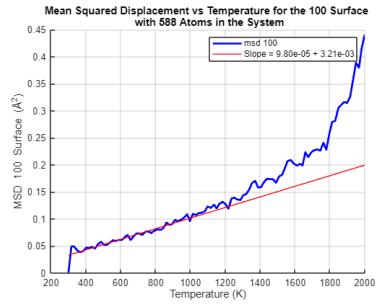
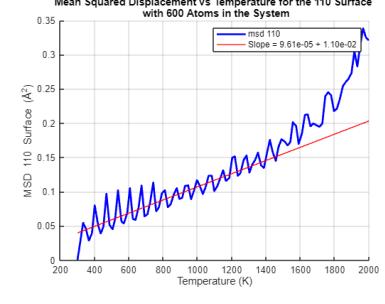
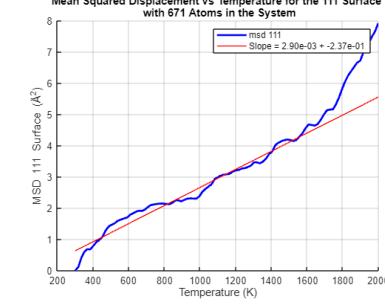
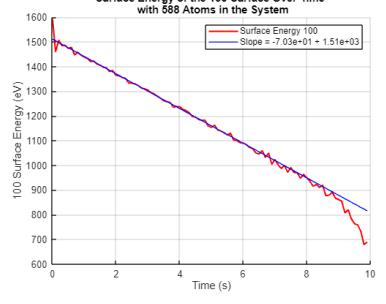
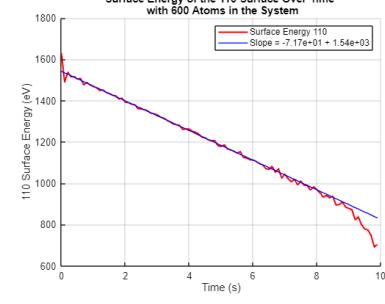
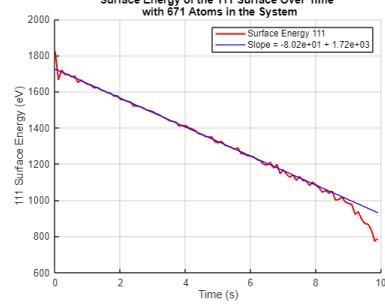
100 Plane of Al	110 Plane of Al	111 Plane of Al
 588 atoms	 600 atoms	 671 atoms
		
Temperature: 1286	Temperature: 1135	Temperature: 1728
Diffusion Constant: $2.451\text{e}+07 \text{ \AA}^2/\text{s}$	Diffusion Constant: $2.404\text{e}+07 \text{ \AA}^2/\text{s}$	Diffusion Constant: $7.245\text{e}+08 \text{ \AA}^2/\text{s}$
		

Table B.4: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=15.92)

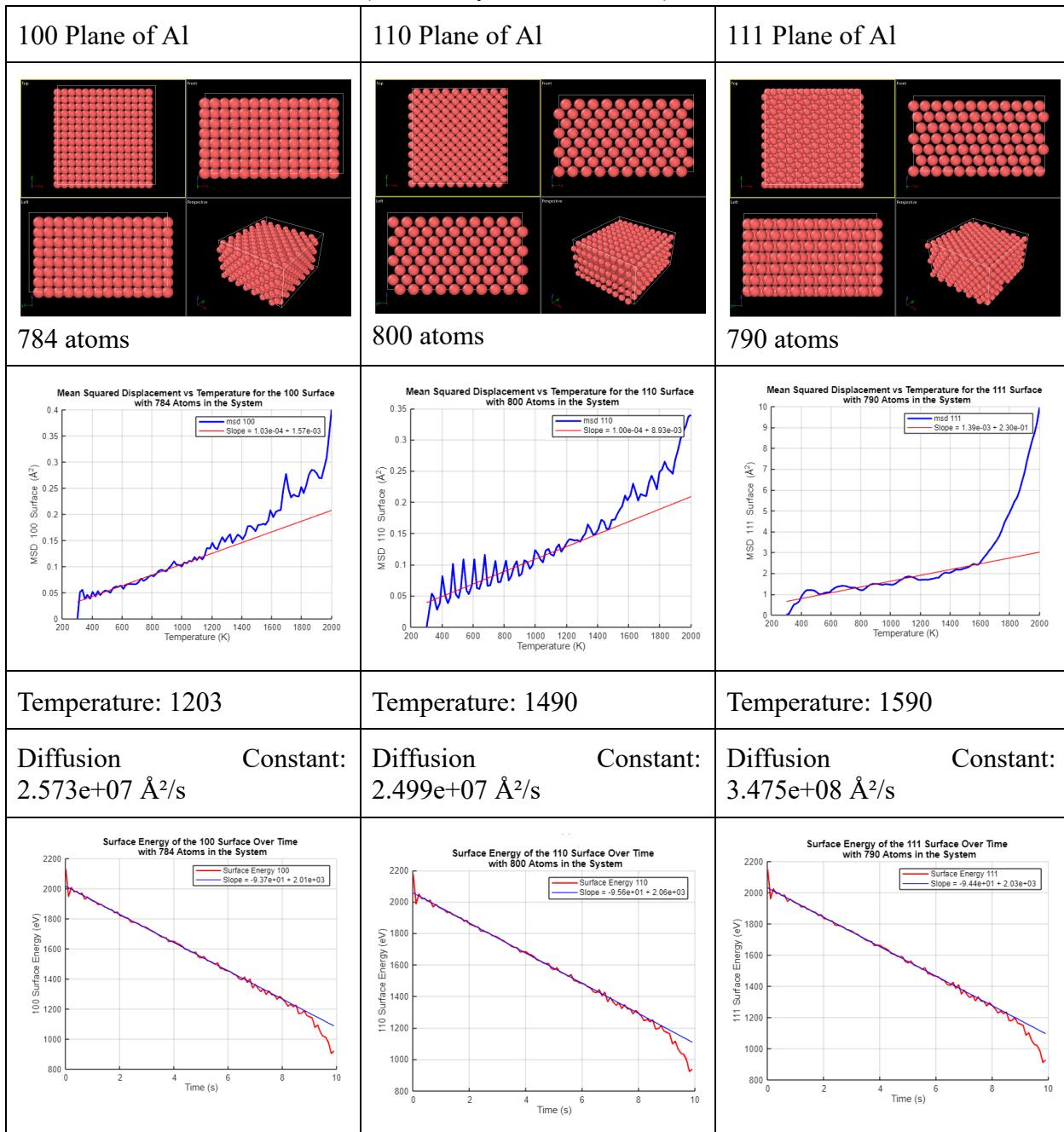


Table B.5: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=19.92)

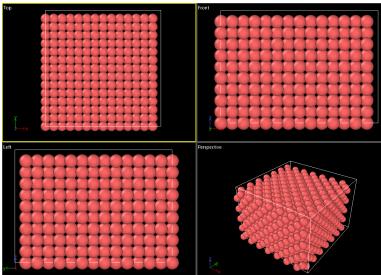
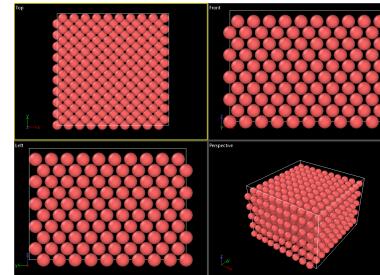
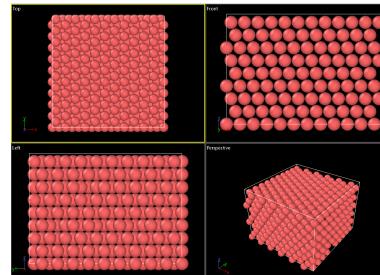
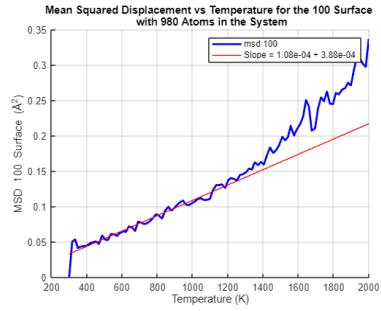
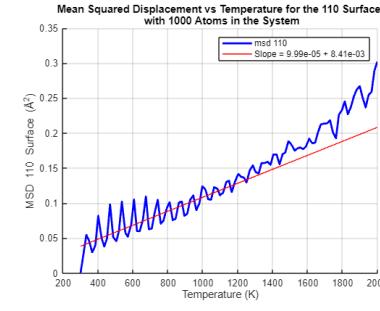
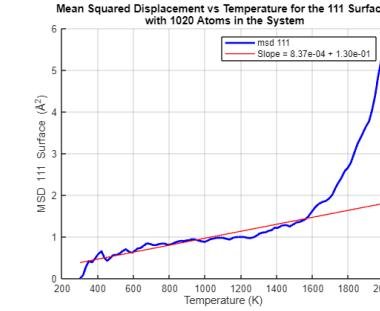
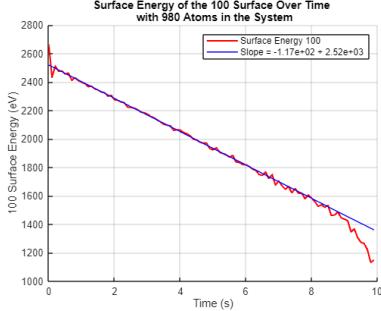
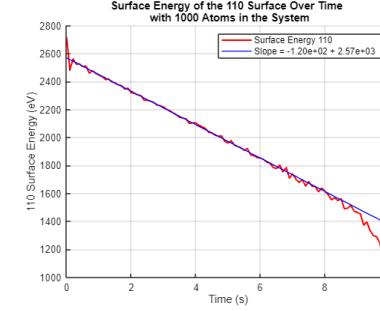
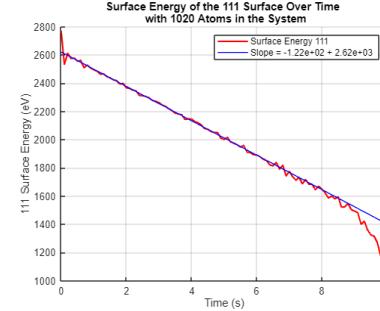
100 Plane of Al	110 Plane of Al	111 Plane of Al
 980 atoms	 1000 atoms	 1020 atoms
		
Temperature: 1371	Temperature: 1422	Temperature: 1556
Diffusion Constant: 2.710e+07 Å²/s	Diffusion Constant: 2.498e+07 Å²/s	Diffusion Constant: 2.092e+08 Å²/s
		

Table B.6: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=23.90)

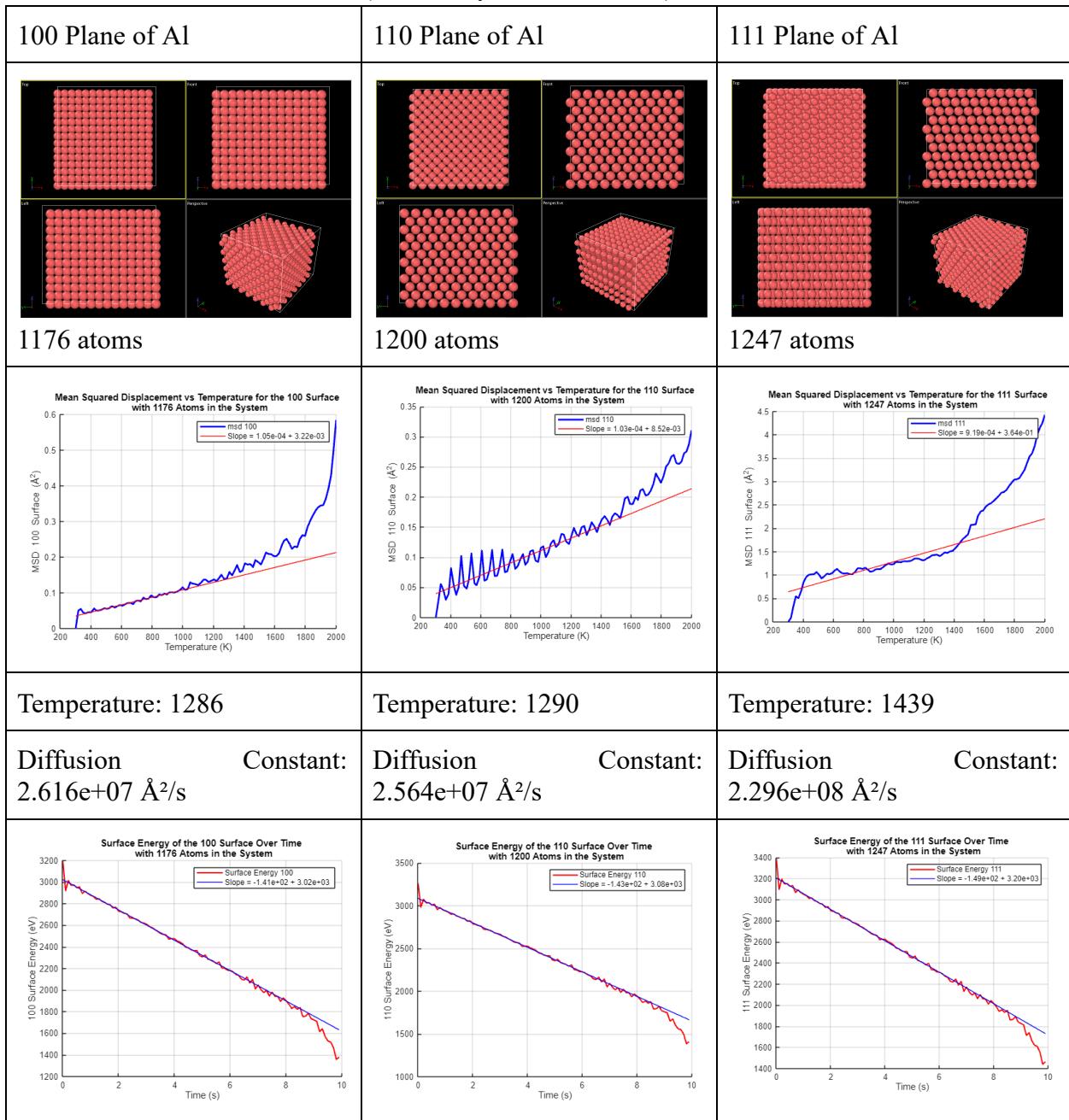


Table B.7: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=27.9)

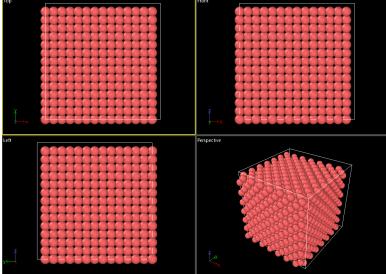
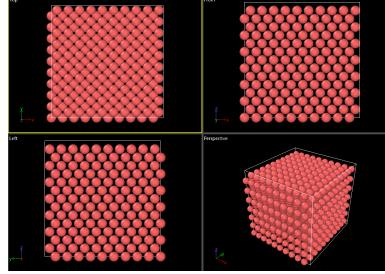
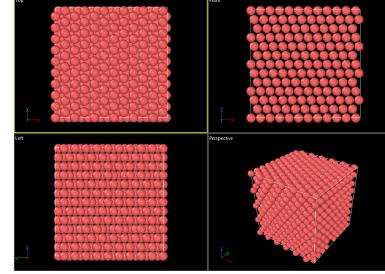
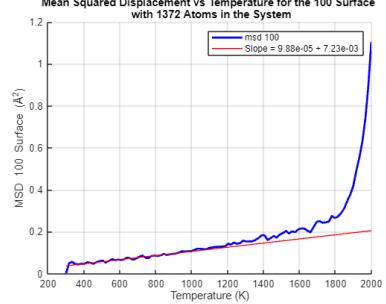
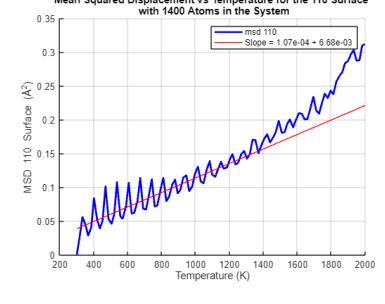
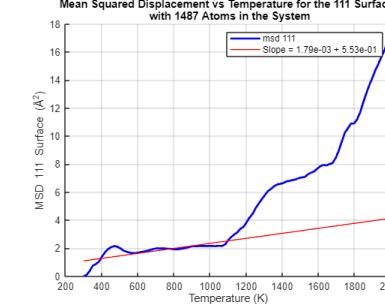
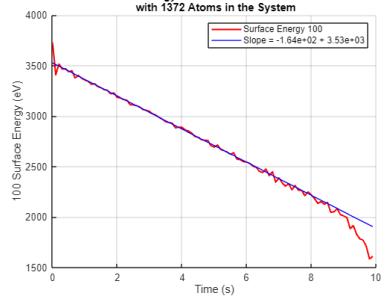
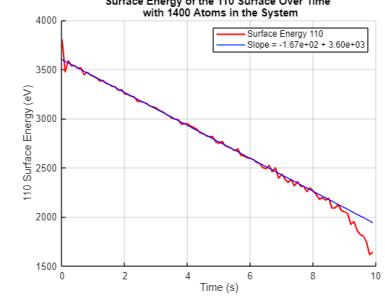
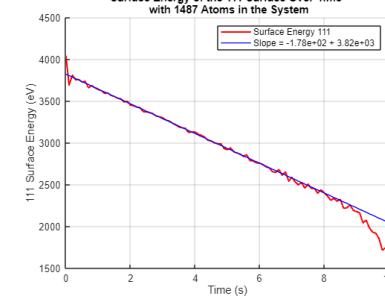
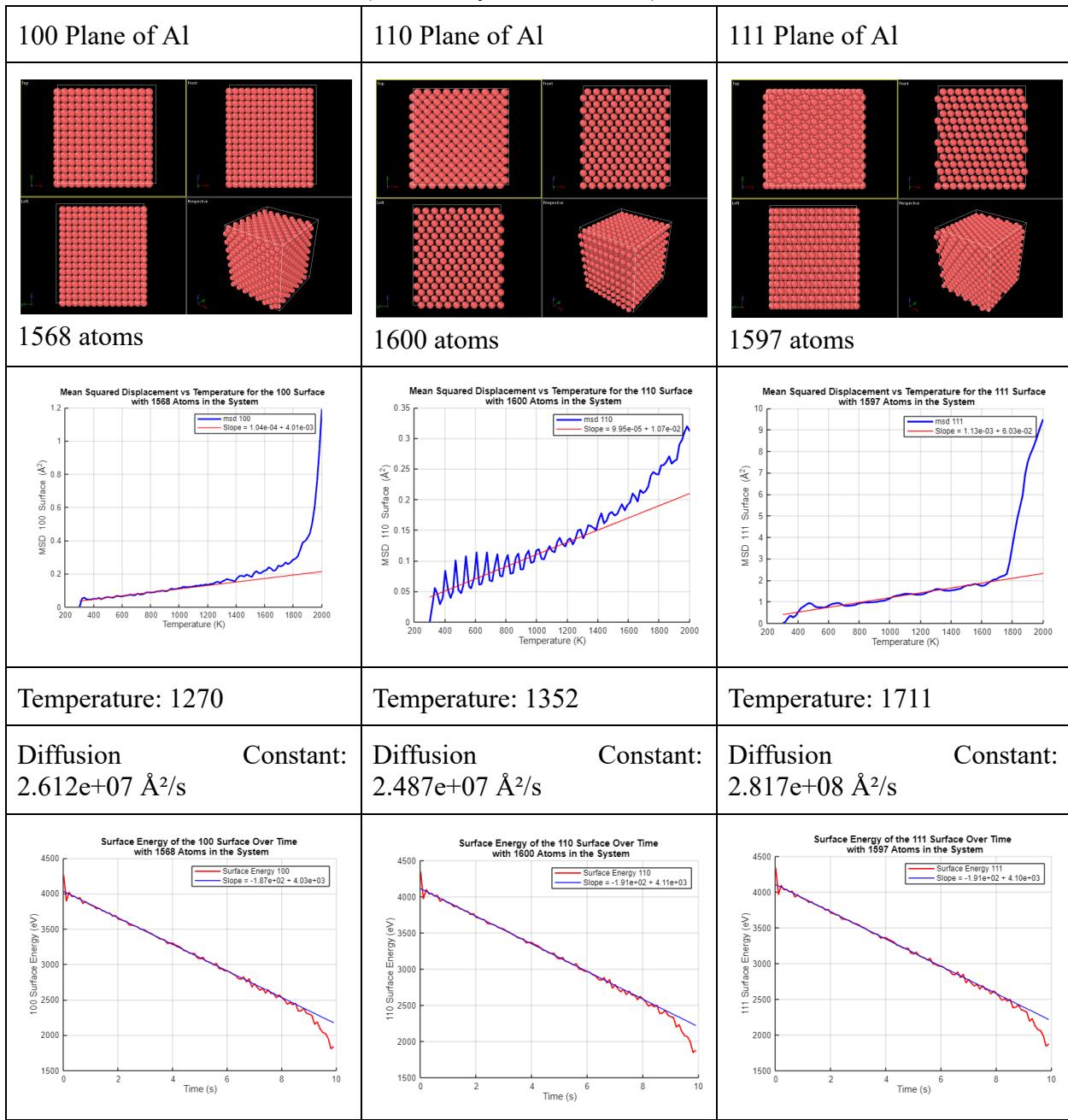
100 Plane of Al	110 Plane of Al	111 Plane of Al
 1372 atoms	 1400 atoms	 1487 atoms
Mean Squared Displacement vs Temperature for the 100 Surface with 1372 Atoms in the System  msd 100 Slope = 9.88e-05 + 7.23e-03	Mean Squared Displacement vs Temperature for the 110 Surface with 1400 Atoms in the System  msd 110 Slope = 1.07e-04 + 6.68e-03	Mean Squared Displacement vs Temperature for the 111 Surface with 1487 Atoms in the System  msd 111 Slope = 1.79e-03 + 5.53e-01
Temperature: 1286	Temperature: 1292	Temperature: 1116
Diffusion Constant: 2.471e+07 Å²/s	Diffusion Constant: 2.682e+07 Å²/s	Diffusion Constant: 4.475e+08 Å²/s
Surface Energy of the 100 Surface Over Time with 1372 Atoms in the System  Surface Energy 100 Slope = -1.64e+02 + 3.53e+03	Surface Energy of the 110 Surface Over Time with 1400 Atoms in the System  Surface Energy 110 Slope = -1.67e+02 + 3.60e-03	Surface Energy of the 111 Surface Over Time with 1487 Atoms in the System  Surface Energy 111 Slope = -1.79e+02 + 3.82e+03

Table B.8: FCC Metal Surfaces: (lx=27.9, ly=27.9, lz=31.9)



Section C: Testing for The Correct Amount of Atoms For Tungsten

Table C.1: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=3.17)

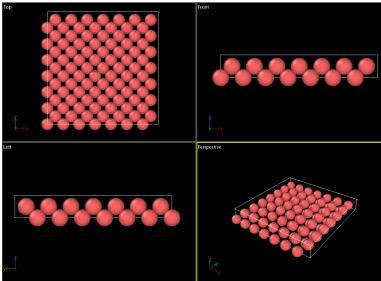
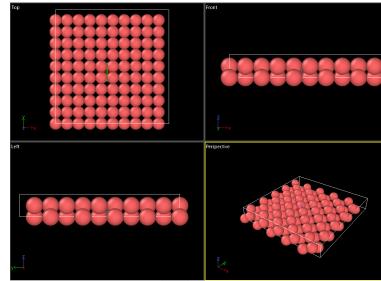
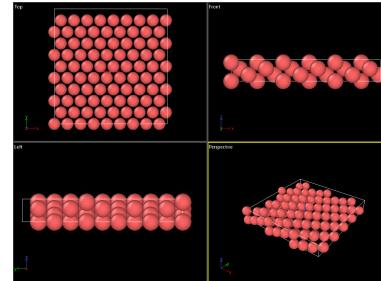
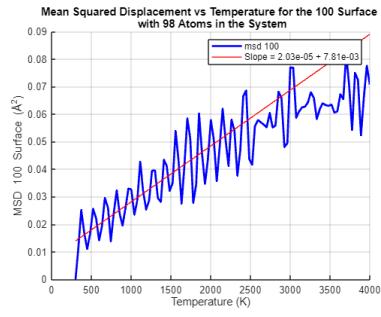
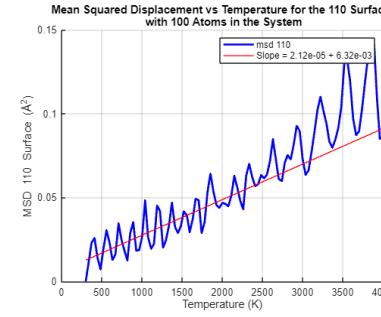
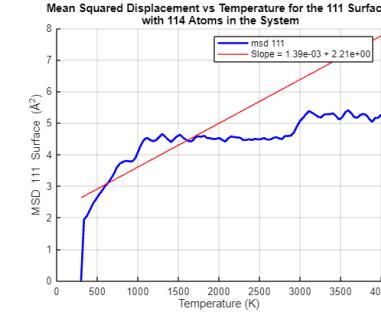
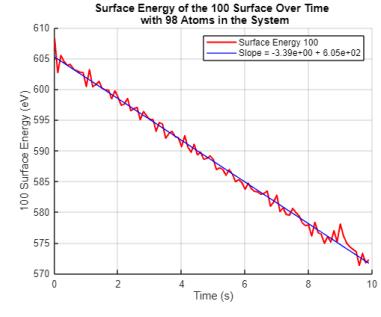
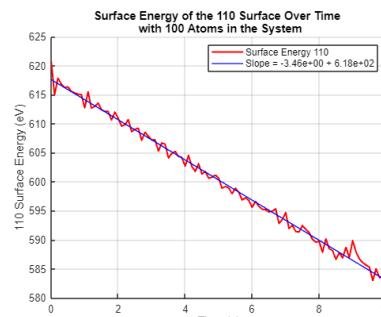
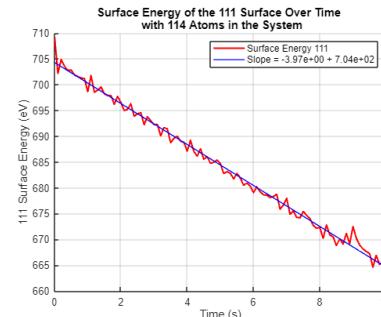
100 Plane of W	110 Plane of W	111 Plane of W
 98 atoms	 100 atoms	 114 atoms
		
Temperature: 3186	Temperature: 3334	Temperature: 3038
Diffusion Constant: $5.072\text{e}+06 \text{ \AA}^2/\text{s}$	Diffusion Constant: $5.295\text{e}+06 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.465\text{e}+08 \text{ \AA}^2/\text{s}$
		

Table C.2: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=6.34)

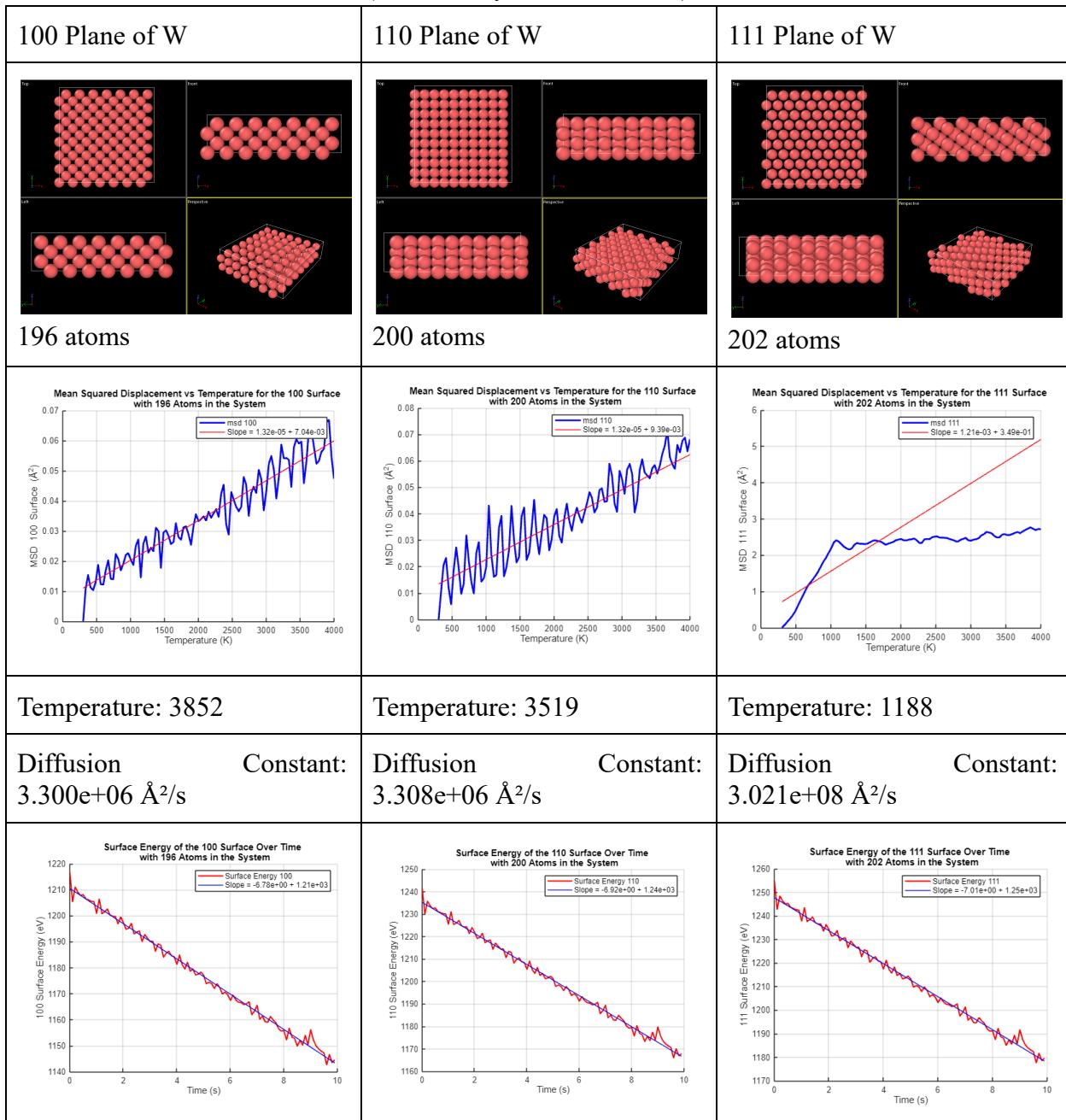


Table C.3: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=9.46)

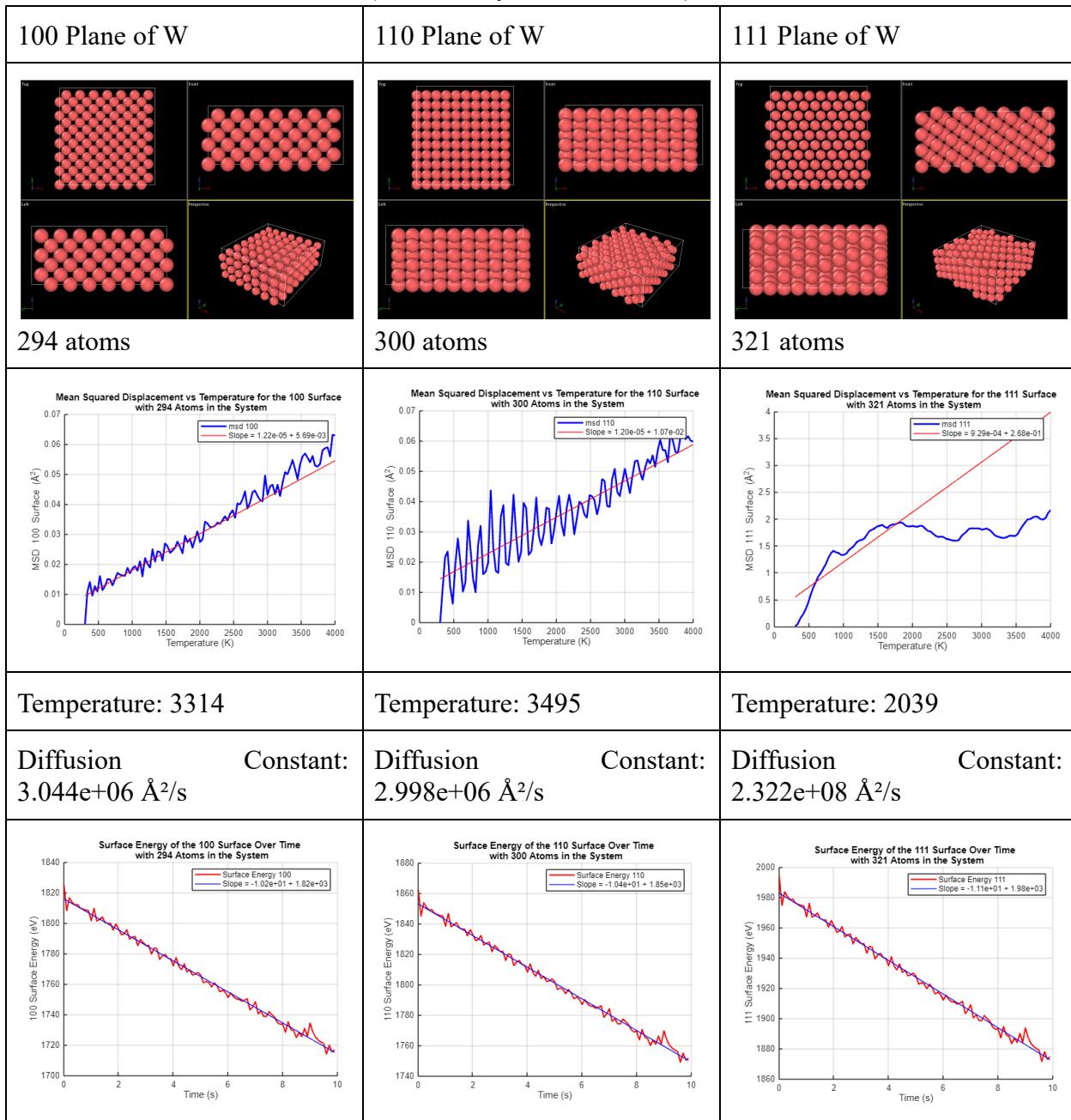


Table C.4: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=12.66)

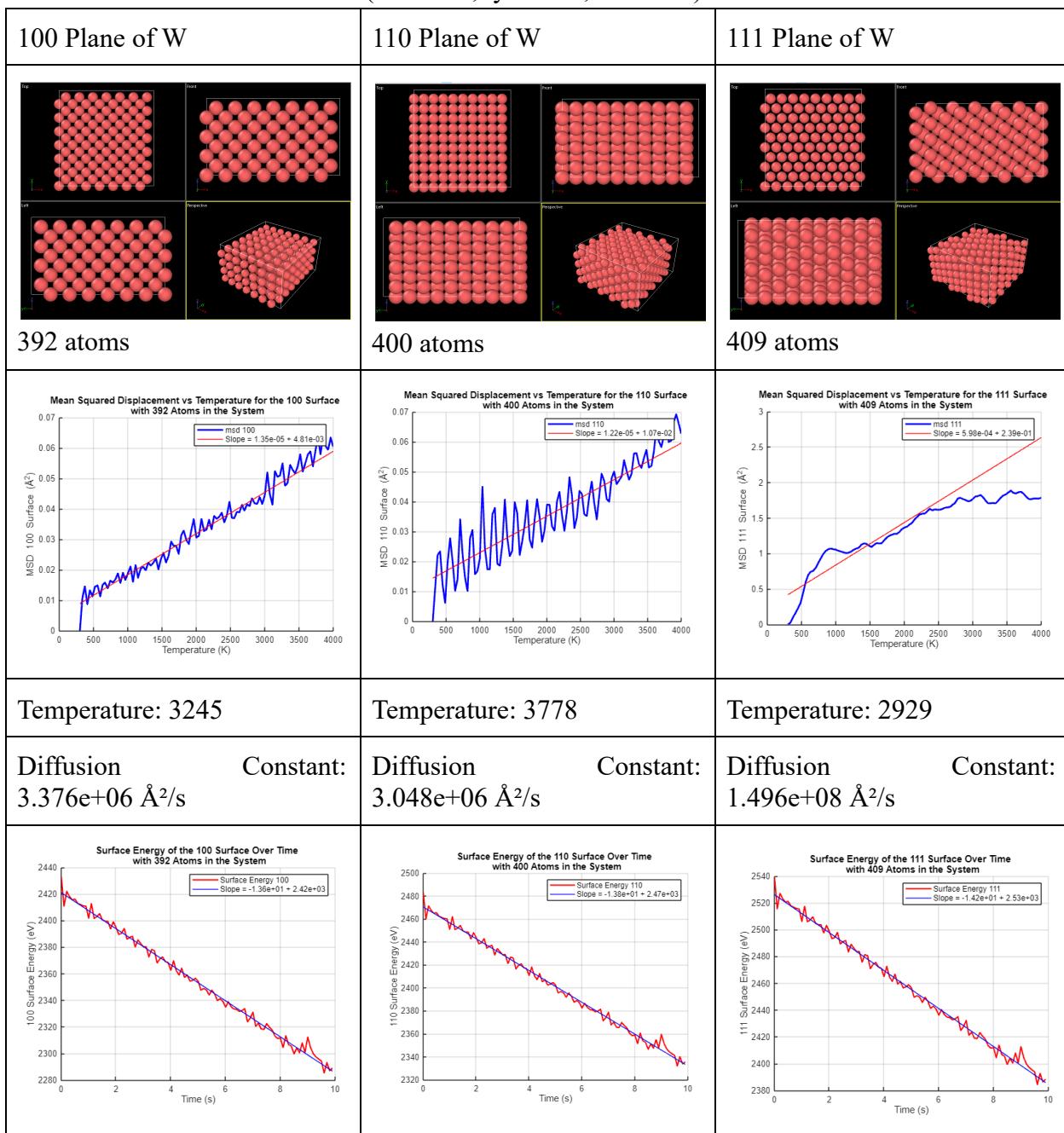


Table C.5: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=15.8)

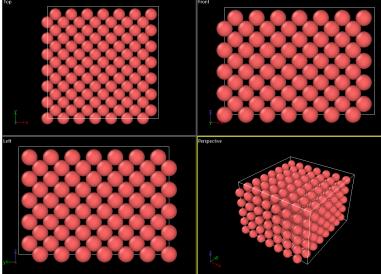
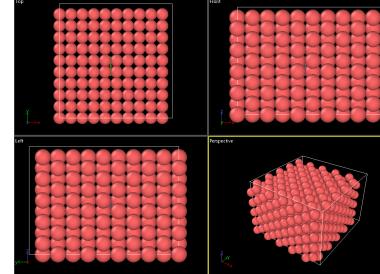
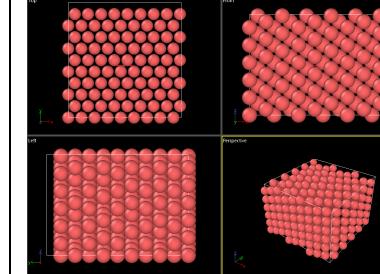
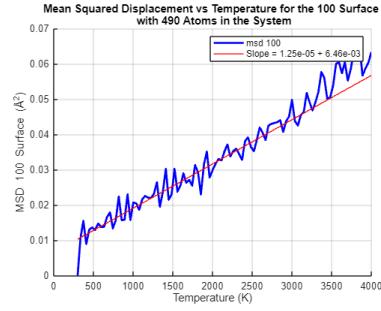
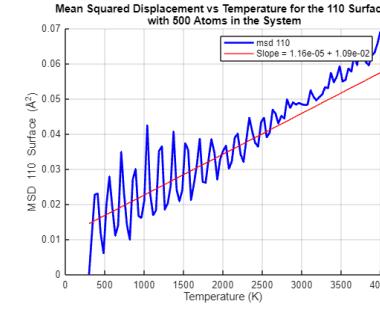
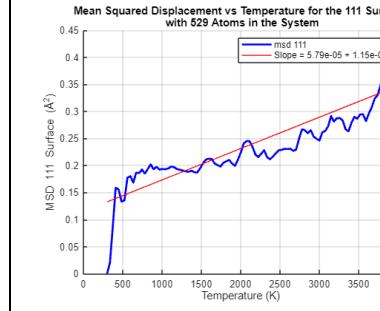
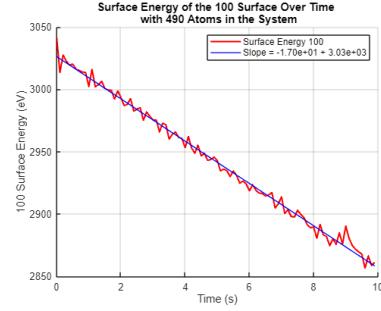
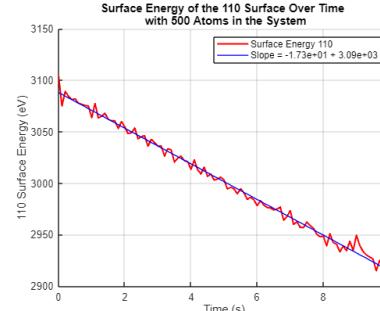
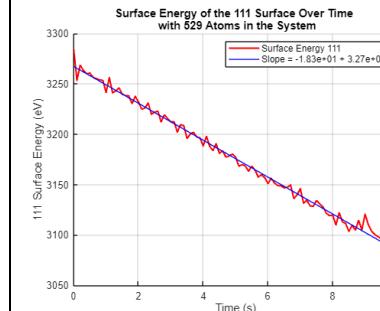
100 Plane of W	110 Plane of W	111 Plane of W
 490 atoms	 500 atoms	 529 atoms
		
Temperature: 3445	Temperature: 2881	Temperature: 3852
Diffusion Constant: 3.136e+06 Å²/s	Diffusion Constant: 2.902e+06 Å²/s	Diffusion Constant: 1.448e+07 Å²/s
		

Table C.6: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=18.9)

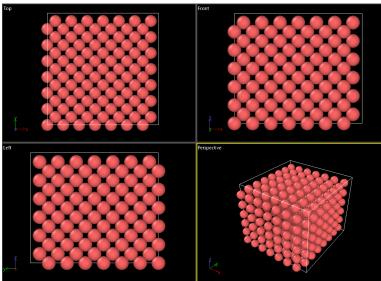
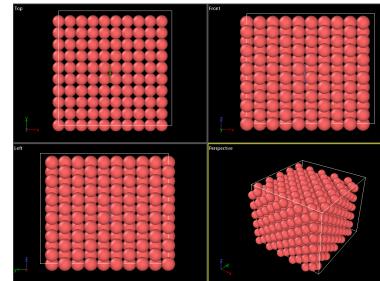
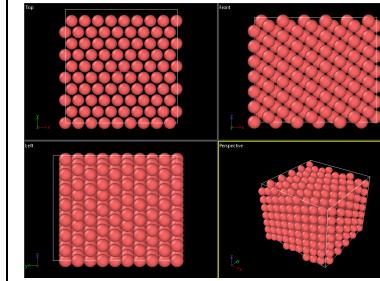
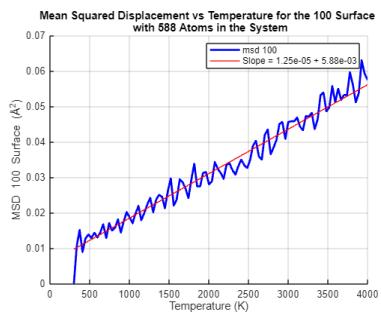
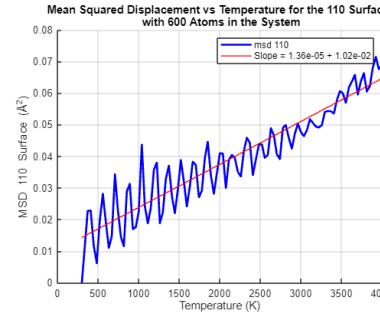
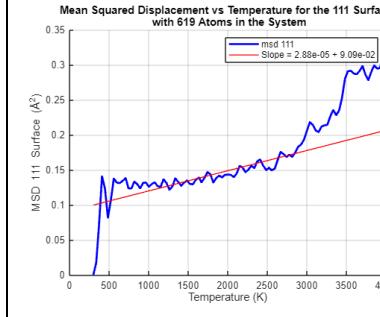
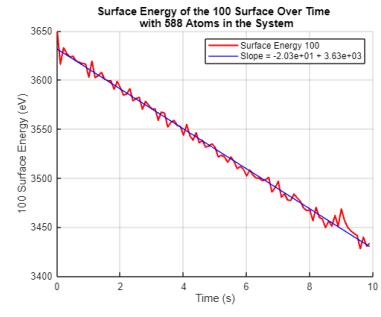
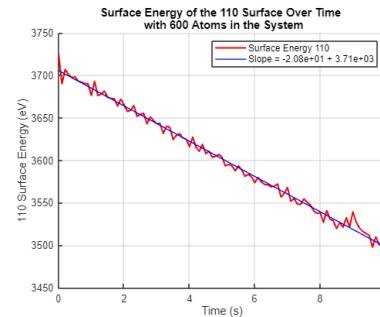
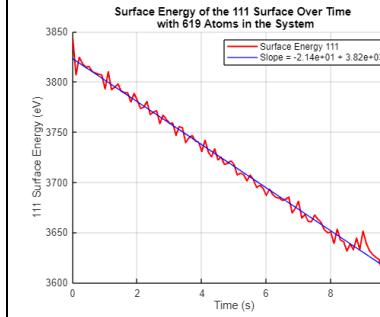
100 Plane of W	110 Plane of W	111 Plane of W
 588 atoms	 600 atoms	 619 atoms
		
Temperature: 3306	Temperature: 3378	Temperature: 3556
Diffusion Constant: $3.134e+06 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.399e+06 \text{ \AA}^2/\text{s}$	Diffusion Constant: $7.211e+08 \text{ \AA}^2/\text{s}$
		

Table C.7: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=22.15)

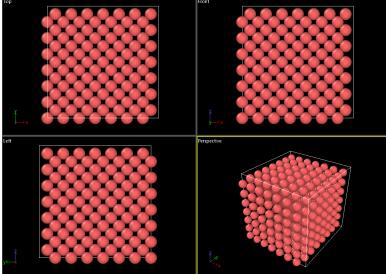
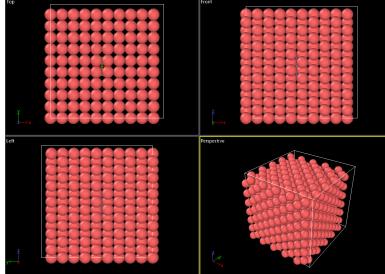
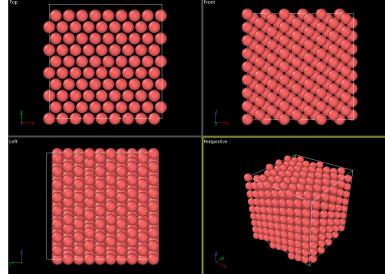
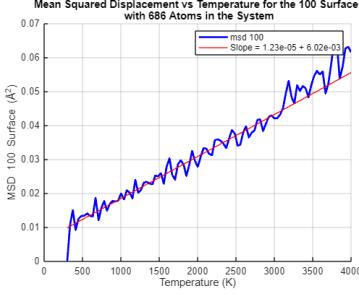
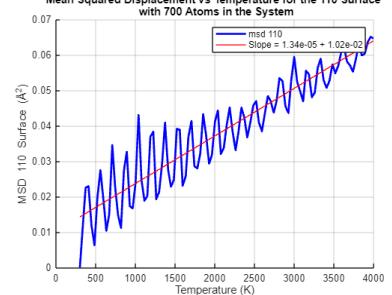
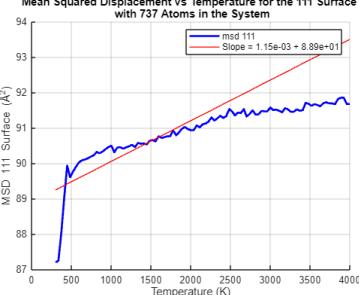
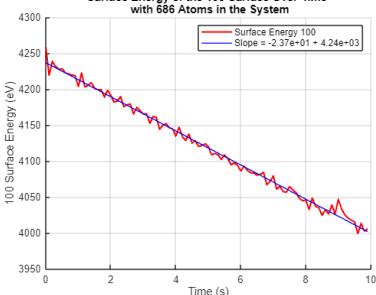
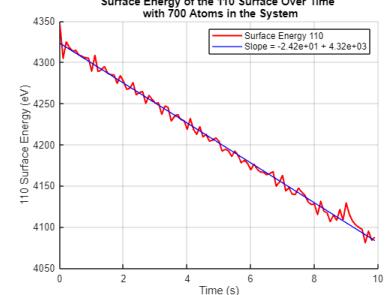
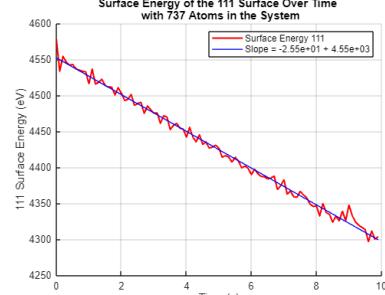
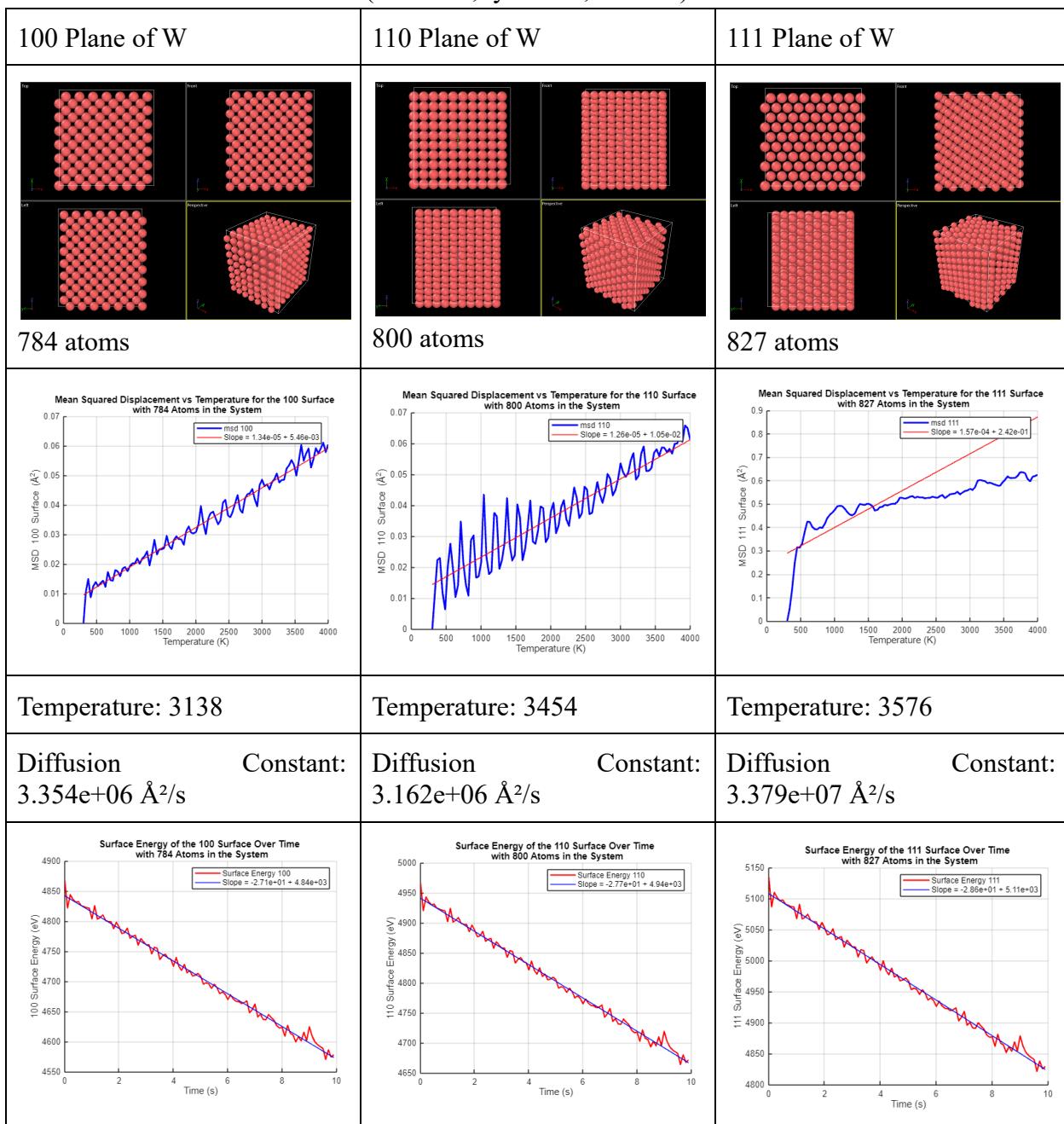
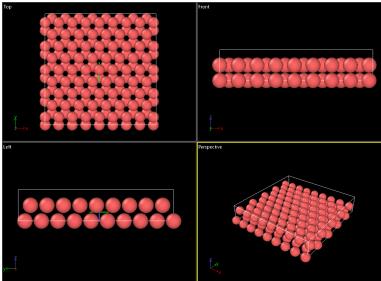
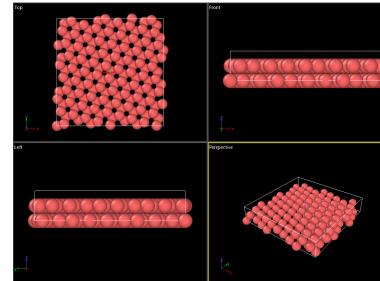
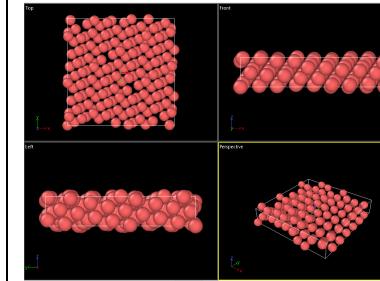
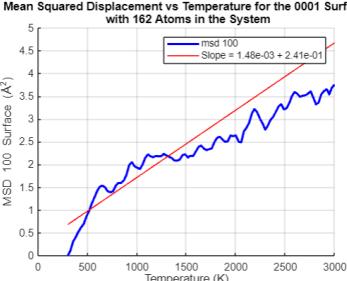
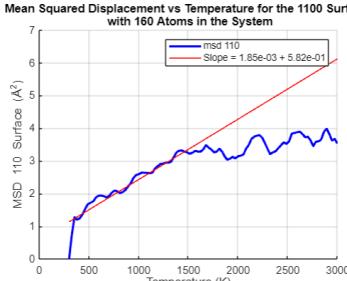
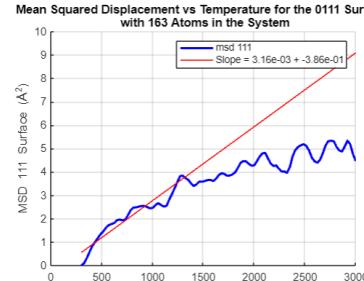
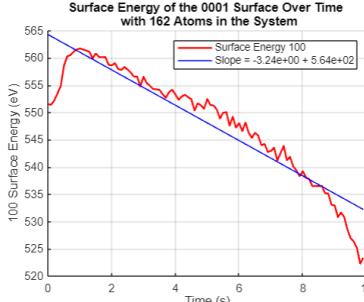
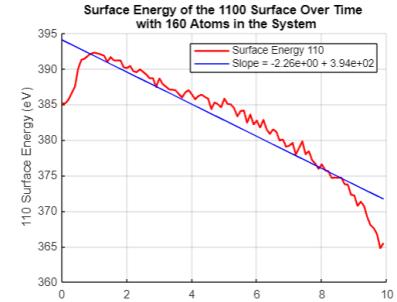
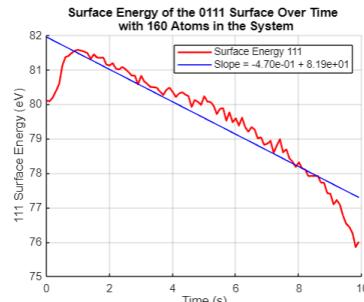
100 Plane of W	110 Plane of W	111 Plane of W
 686 atoms	 700 atoms	 737 atoms
		
Temperature: 3097	Temperature: 3566	Temperature: 3457
Diffusion Constant: $3.087\text{e}+06 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.354\text{e}+06 \text{ \AA}^2/\text{s}$	Diffusion Constant: $2.871\text{e}+08 \text{ \AA}^2/\text{s}$
		

Table C.8: BCC Metal Surfaces: (lx=22.16, ly=22.16, lz=25.2)

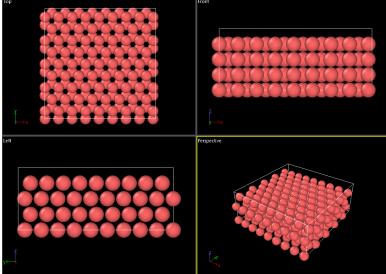
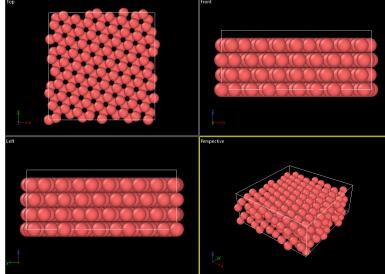
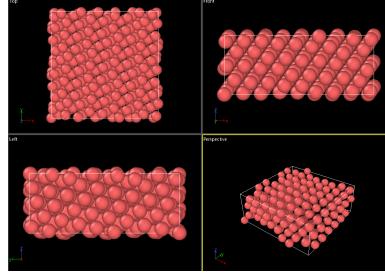
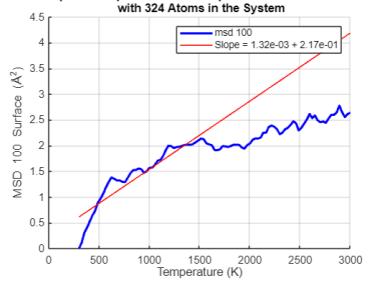
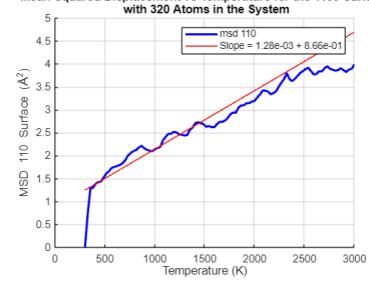
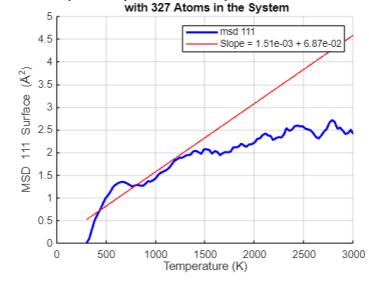
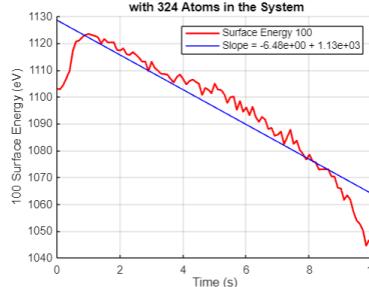
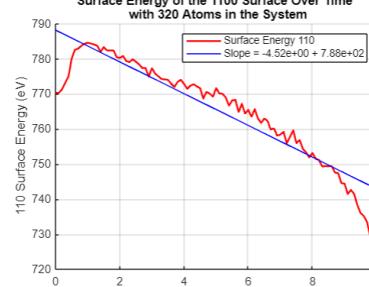
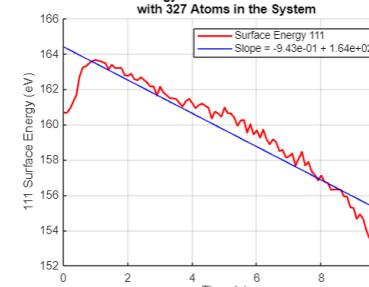


Section D: Testing for The Correct Amount of Atoms For Titanium

Table D.1: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=4.8)

0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 162 atoms	 160 atoms	 163 atoms
Mean Squared Displacement vs Temperature for the 0001 Surface with 162 Atoms in the System 	Mean Squared Displacement vs Temperature for the 1100 Surface with 160 Atoms in the System 	Mean Squared Displacement vs Temperature for the 0111 Surface with 163 Atoms in the System 
Temperature: 2163	Temperature: 2134	Temperature: 2352
Diffusion Constant: $3.692\text{e+}08 \text{ \AA}^2/\text{s}$	Diffusion Constant: $4.616\text{e+}08 \text{ \AA}^2/\text{s}$	Diffusion Constant: $7.895\text{e+}08 \text{ \AA}^2/\text{s}$
Surface Energy of the 0001 Surface Over Time with 162 Atoms in the System 	Surface Energy of the 1100 Surface Over Time with 160 Atoms in the System 	Surface Energy of the 0111 Surface Over Time with 163 Atoms in the System 

Tabel D.2: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=9.63)

0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 324 atoms	 320 atoms	 327 atoms
Mean Squared Displacement vs Temperature for the 0001 Surface with 324 Atoms in the System 	Mean Squared Displacement vs Temperature for the 1100 Surface with 320 Atoms in the System 	Mean Squared Displacement vs Temperature for the 0111 Surface with 327 Atoms in the System 
Temperature: 2082	Temperature: 2207	Temperature: 2198
Diffusion Constant: $3.308e+08 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.188e+08 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.763e+08 \text{ \AA}^2/\text{s}$
Surface Energy of the 0001 Surface Over Time with 324 Atoms in the System 	Surface Energy of the 1100 Surface Over Time with 320 Atoms in the System 	Surface Energy of the 0111 Surface Over Time with 327 Atoms in the System 

Tabel D.3: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=14.45)

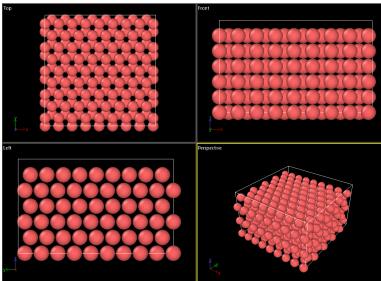
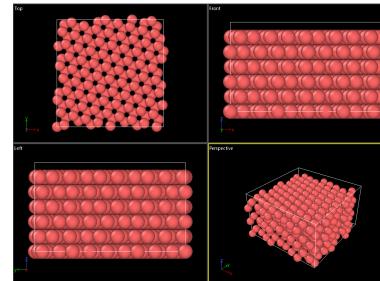
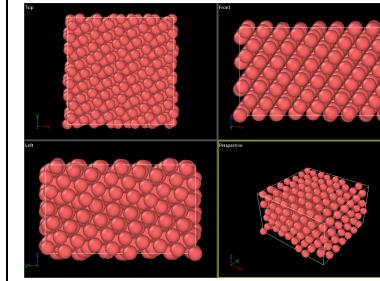
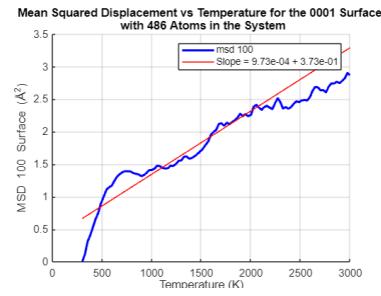
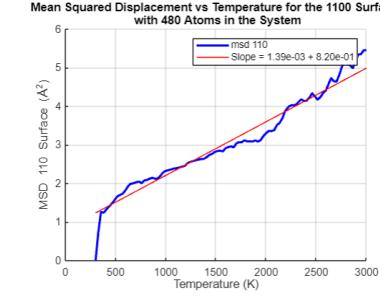
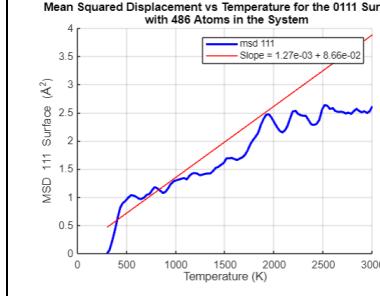
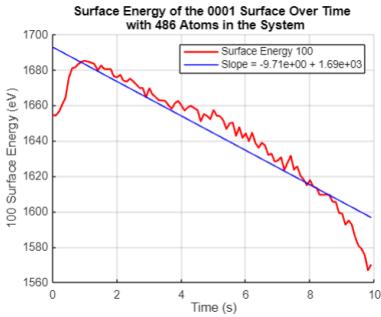
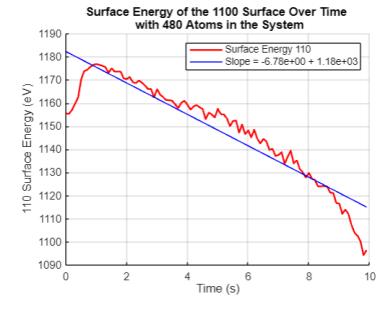
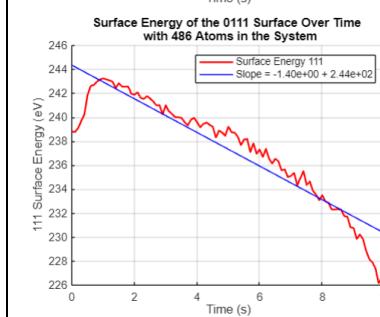
0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 486 atoms	 480 atoms	 486 atoms
		
Temperature: 1572	Temperature: 2132	Temperature: 1674
Diffusion Constant: 2.432e+08 Å²/s	Diffusion Constant: 3.472e+08 Å²/s	Diffusion Constant: 3.163e+08 Å²/s
		

Table D.4: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=19.27)

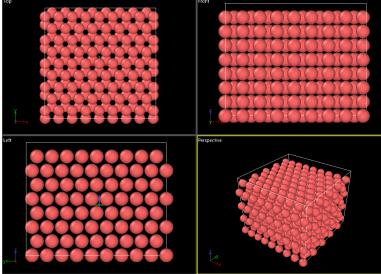
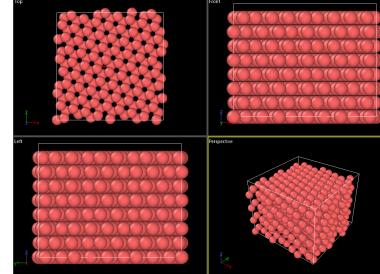
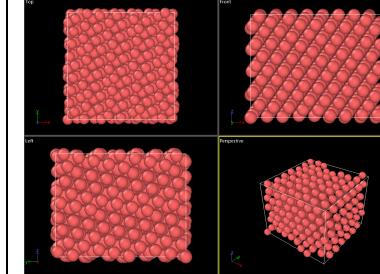
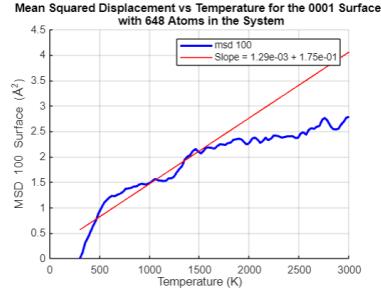
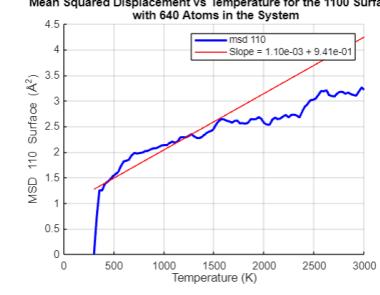
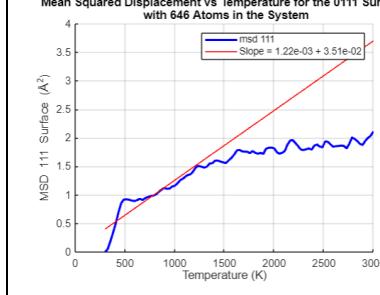
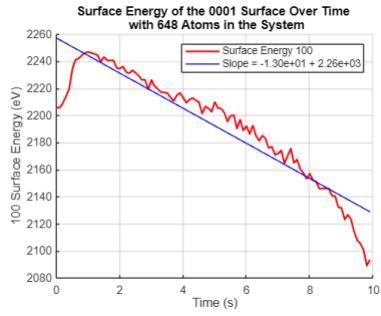
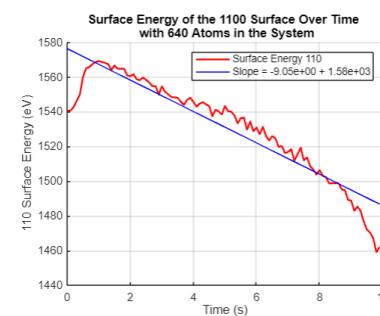
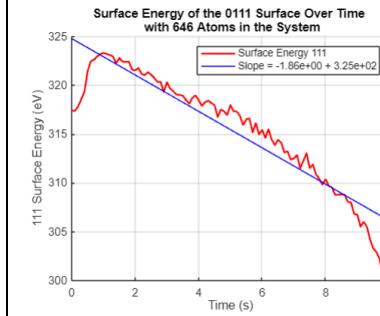
0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 648 atoms	 640 atoms	 646 atoms
		
Temperature: 1346	Temperature: 1413	Temperature: 1532
Diffusion Constant: $3.235\text{e}+08 \text{ Å}^2/\text{s}$	Diffusion Constant: $2.754\text{e}+08 \text{ Å}^2/\text{s}$	Diffusion Constant: $3.054\text{e}+08 \text{ Å}^2/\text{s}$
		

Table D.5: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=24.1)

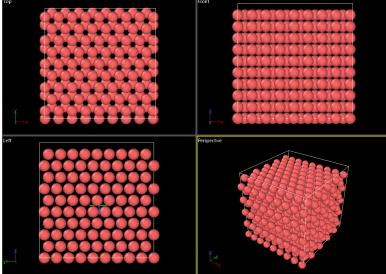
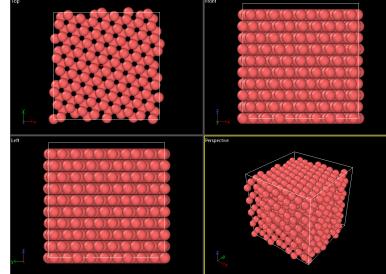
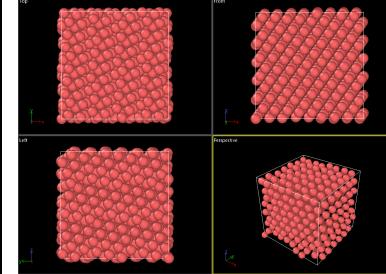
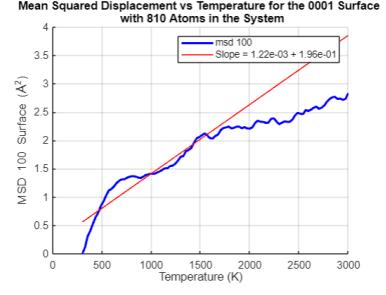
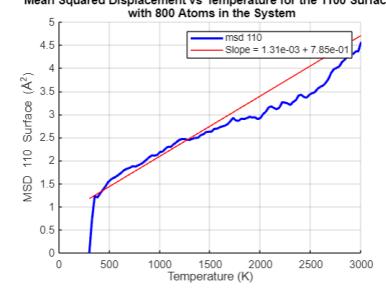
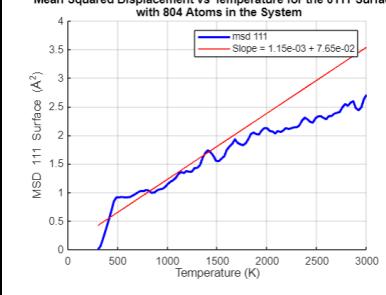
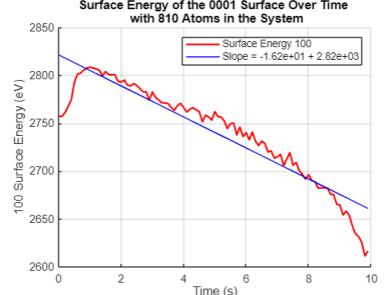
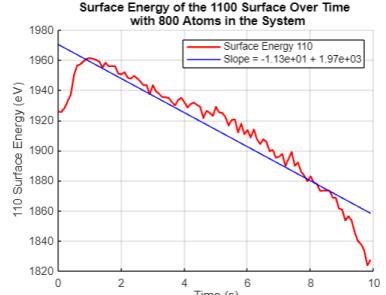
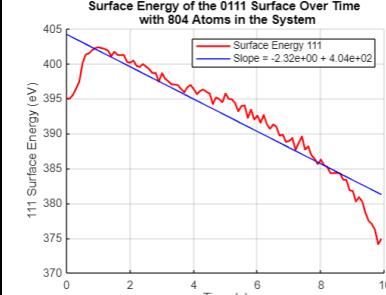
0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 810 atoms	 800 atoms	 804 atoms
 Temperature: 1403	 Temperature: 1624	 Temperature: 1326
Diffusion Constant: $3.048 \times 10^8 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.267 \times 10^8 \text{ \AA}^2/\text{s}$	Diffusion Constant: $2.887 \times 10^8 \text{ \AA}^2/\text{s}$
		

Table D.6: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=29.0)

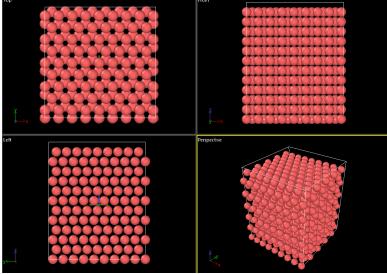
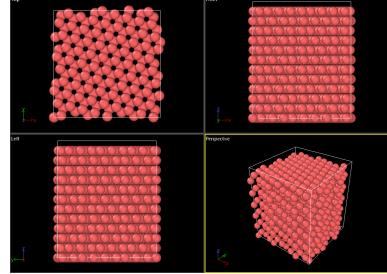
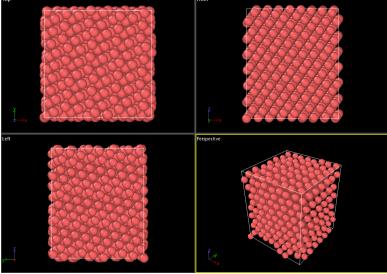
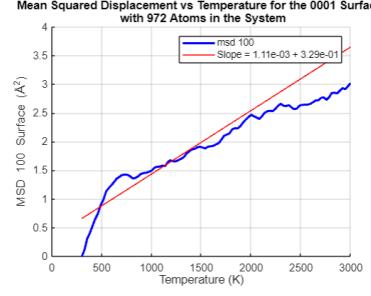
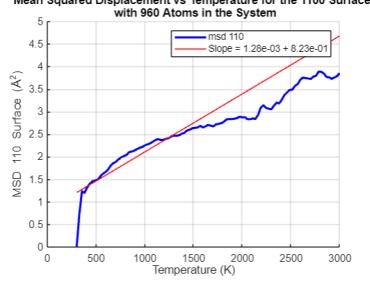
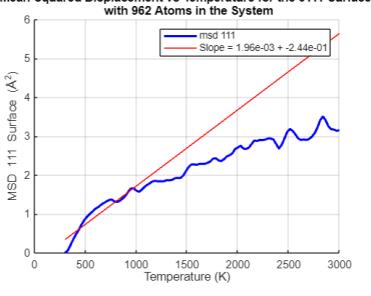
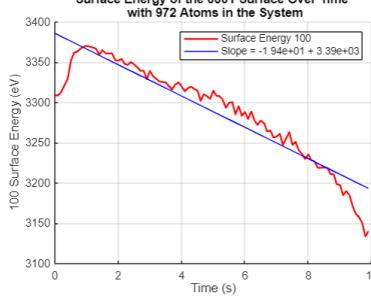
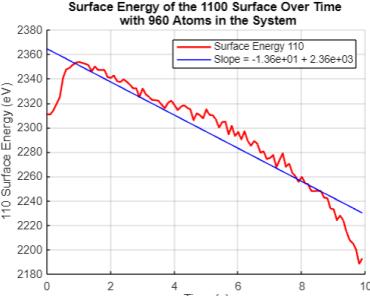
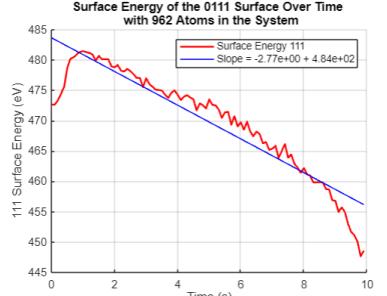
0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 972 atoms	 960 atoms	 962 atoms
Mean Squared Displacement vs Temperature for the 0001 Surface with 972 Atoms in the System  MSD 100 Slope = 1.11e-03 + 3.29e-01	Mean Squared Displacement vs Temperature for the 1100 Surface with 960 Atoms in the System  MSD 110 Slope = 1.28e-03 + 8.23e-01	Mean Squared Displacement vs Temperature for the 0111 Surface with 962 Atoms in the System  MSD 111 Slope = 1.96e-03 + -2.44e-01
Temperature: 1783	Temperature: 1568	Temperature: 1495
Diffusion Constant: 2.767e+08 Å²/s	Diffusion Constant: 3.212e+08 Å²/s	Diffusion Constant: 4.904e+08 Å²/s
Surface Energy of the 0001 Surface Over Time with 972 Atoms in the System  100 Surface Energy (eV) Slope = -1.94e+01 + 3.39e+03	Surface Energy of the 1100 Surface Over Time with 960 Atoms in the System  110 Surface Energy (eV) Slope = -1.36e+01 + 2.36e+03	Surface Energy of the 0111 Surface Over Time with 962 Atoms in the System  111 Surface Energy (eV) Slope = -2.77e+00 + 4.84e+02

Table D.7: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=33.8)

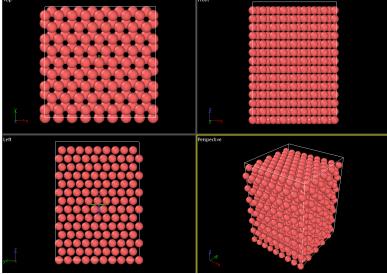
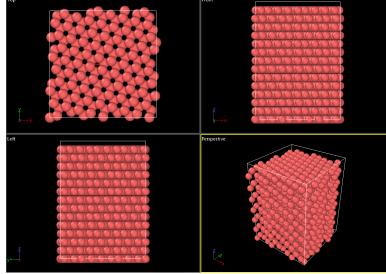
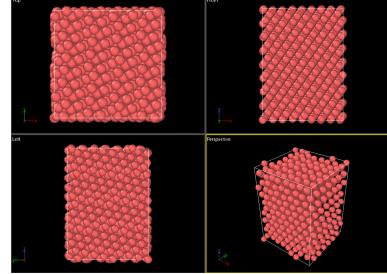
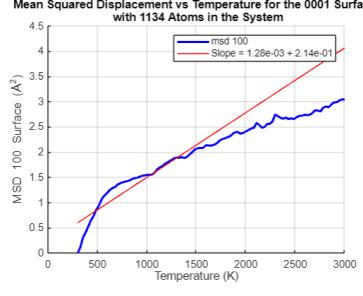
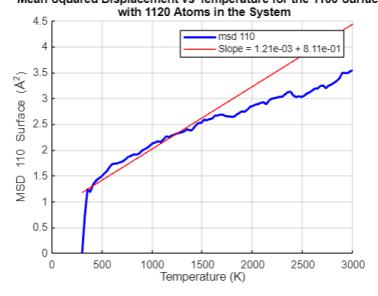
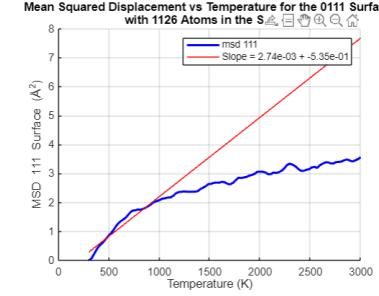
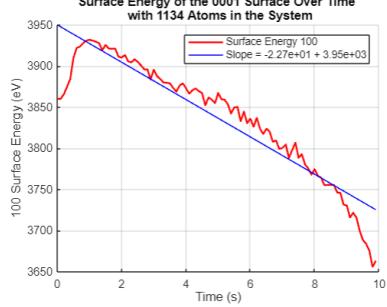
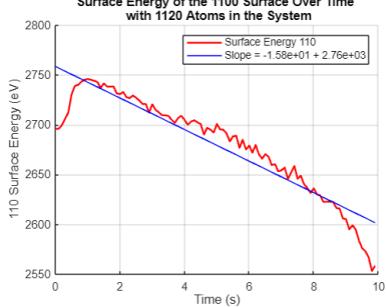
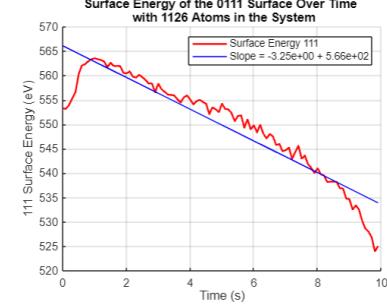
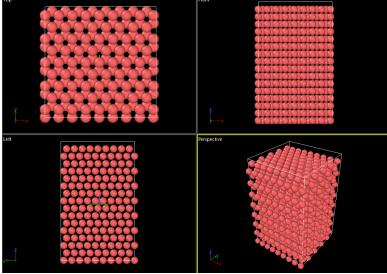
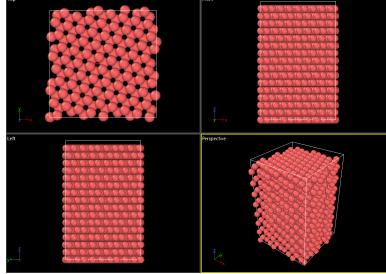
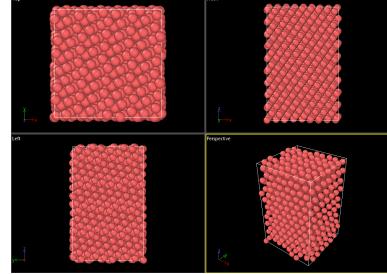
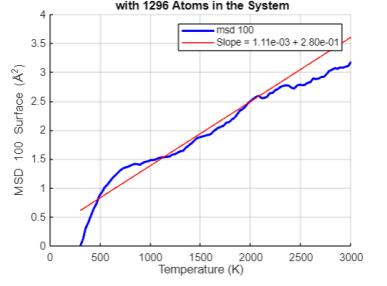
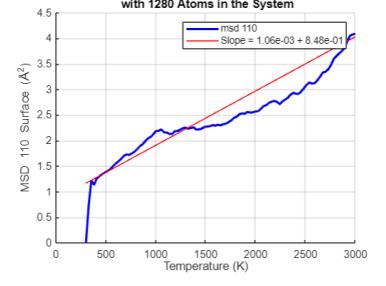
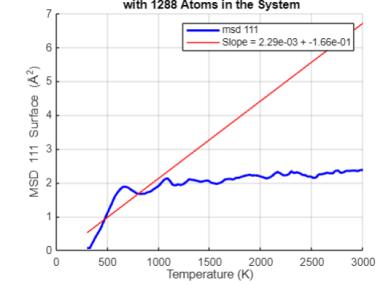
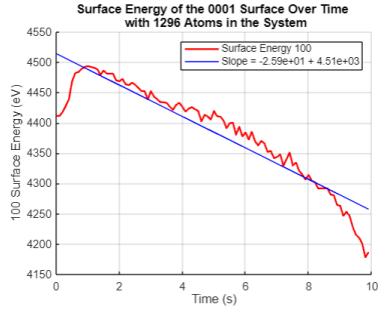
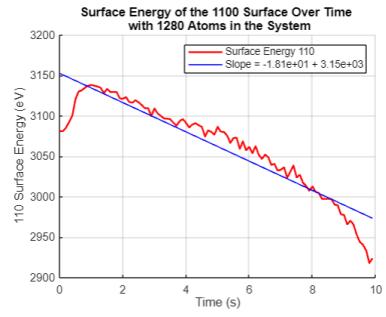
0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 1134 atoms	 1120 atoms	 1126 atoms
		
Temperature: 1456	Temperature: 1675	Temperature: 1564
Diffusion Constant: $3.206 \times 10^8 \text{ \AA}^2/\text{s}$	Diffusion Constant: $3.023 \times 10^8 \text{ \AA}^2/\text{s}$	Diffusion Constant: $6.841 \times 10^8 \text{ \AA}^2/\text{s}$
		

Table D.8: HCP Metal Surfaces: (lx=24.6, ly=24.6, lz=38.6)

0001 Plane of Ti	1100 Plane of Ti	0111 Plane of Ti
 1296 atoms	 1280 atoms	 1288 atoms
Mean Squared Displacement vs Temperature for the 0001 Surface with 1296 Atoms in the System 	Mean Squared Displacement vs Temperature for the 1100 Surface with 1280 Atoms in the System 	Mean Squared Displacement vs Temperature for the 0111 Surface with 1288 Atoms in the System 
Temperature: 2289	Temperature: 2201	Temperature: 953
Diffusion Constant: $2.772e+08 \text{ \AA}^2/\text{s}$	Diffusion Constant: $2.650e+08 \text{ \AA}^2/\text{s}$	Diffusion Constant: $5.735e+08 \text{ \AA}^2/\text{s}$
Surface Energy of the 0001 Surface Over Time with 1296 Atoms in the System 	Surface Energy of the 1100 Surface Over Time with 1280 Atoms in the System 	Surface Energy of the 0111 Surface Over Time with 1288 Atoms in the System 