MSE 203 - Introduction to Computational Materials Engineering
Thin Film Deposition of Si on a Substrate

Group Members

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Abstract:

Thin film deposition of silicon (Si) onto substrates is a fundamental process in materials engineering, with applications spanning from semiconductor device fabrication to flexible electronics and biomedical implants. This project explores the computational aspects of simulating silicon thin film deposition on crystalline silicon substrates using the LAMMPS molecular dynamics software. Through simulations, we investigate the structural and mechanical properties of the deposited films, focusing on factors such as deposition energy, substrate temperature, and post-deposition annealing. By understanding the atomistic mechanisms governing thin film growth, we aim to contribute to the optimization of deposition processes and the design of advanced materials for various technological applications.

Introduction :-

Thin film deposition of silicon (Si) onto substrates is a common process in materials engineering. It involves coating a surface with a thin layer of silicon using methods like chemical or physical vapor deposition. This technique is crucial in making semiconductor devices like microchips and solar cells, where silicon layers play essential roles. Beyond electronics, thin silicon films find use in flexible electronics, sensors, and medical devices.

Understanding how silicon thin films are deposited helps engineers control film properties and improve device performance. Through computer simulations and experiments, researchers explore the details of this process. This project focuses on simulating silicon thin film deposition to understand how it works at the molecular level. By studying this, we aim to contribute to the development of better materials and devices for various applications.

Deposition Energy :-

$$E = \frac{1}{2}mv^2$$

where $m = 4.67 \times 10^{-26}$ kg/atom and $v = 2 \times 10^3$ m/s,

$$E = \frac{1}{2} \times (4.67 \times 10^{-26} \text{ kg/atom}) \times (2 \times 10^3 \text{ m/s})^2$$

$$E = 9.34 \times 10^{-20} \text{ J}$$

Converting to eV ($1 \text{ eV} = 1.602 \times 10^{-19}$ J), we get:

$$\text{Deposition energy} = \frac{9.34 \times 10^{-20} \text{ J}}{1.602 \times 10^{-19} \text{ J/eV}} = 0.583 \text{ eV}$$

Thin film Deposition Simulation and Characterization :

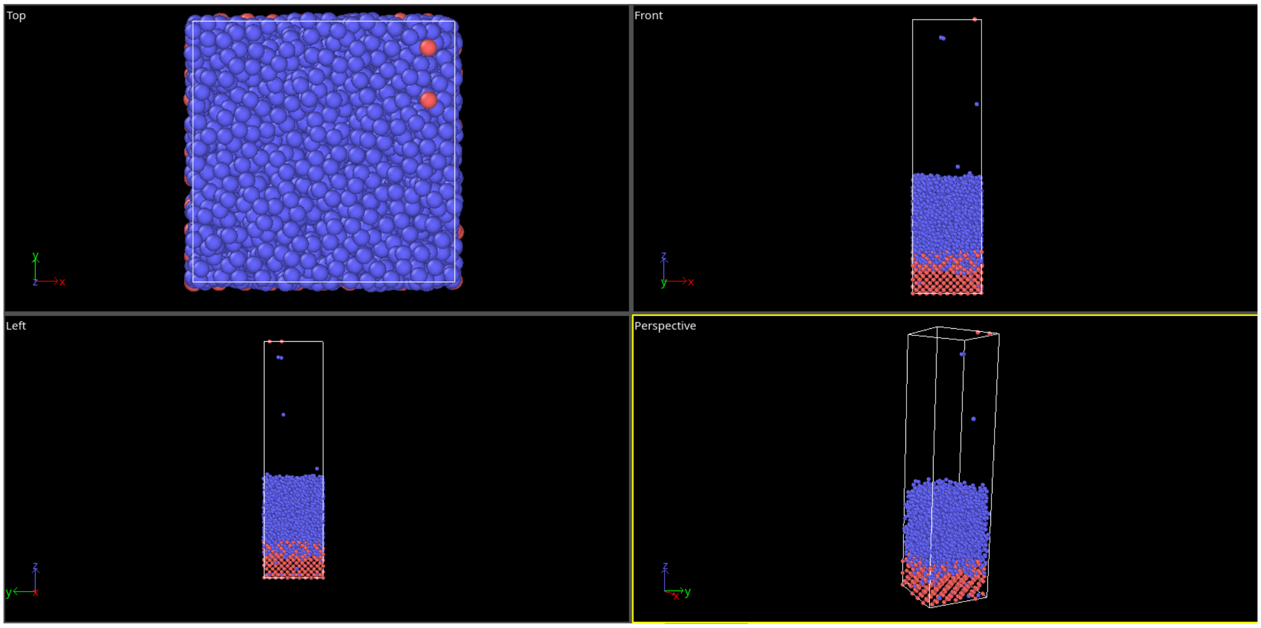


Fig 1: End result of simulation of thin film deposition of Si

The red atoms in fig 1 are the substrate atoms and the blue colored atoms are the deposited silicon atoms. The blue atoms collectively make thin film. The substrate is made of 650 Si atoms and the film is made up of a total of 3000 Si atoms.

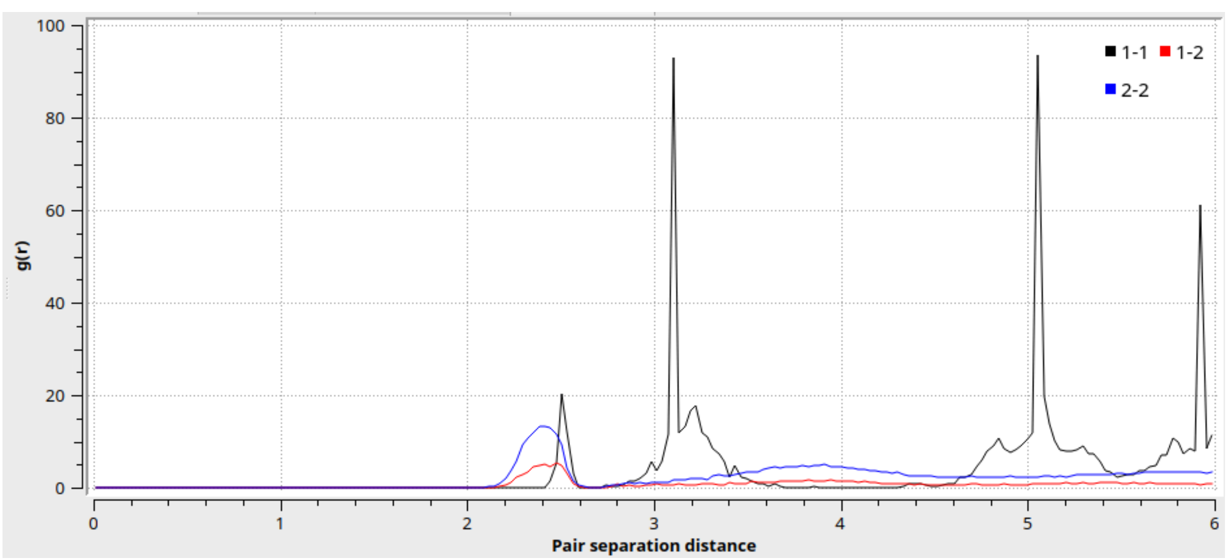


Fig 2 : Partial RDF plot. The black plot is for substrate and blue is for the deposited film

From fig 2, it can be observed that the blue plot, which is a partial RDF plot for thin film, shows a single broad peak indicating amorphous character of the film.

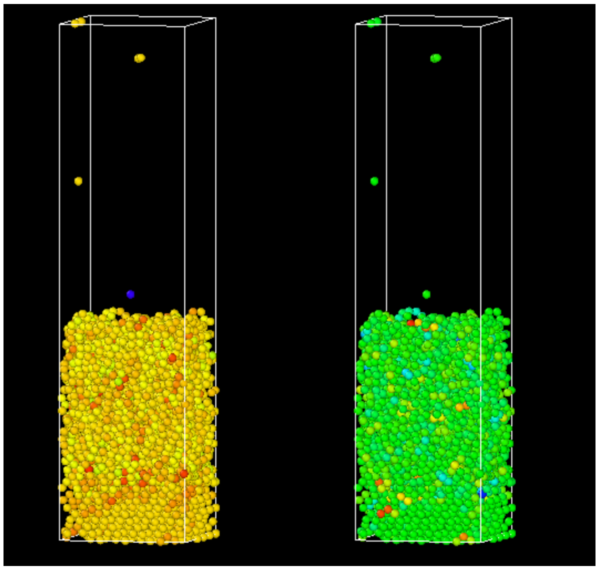


Fig 3: End simulation color coded based on (a) longitudinal stress (to the left) and (b) transversal stress at 300k (to the right)

(color coded based on VIBGYOR. Stress values increases from Violet to Red)

From Fig 3(a), it can be seen that the substrate atoms have a slightly more longitudinal stress compared to the deposited atoms as their color is slightly darker than that of deposited atoms. This is because of force being applied on the substrate atoms by the deposited atoms. Whereas, the transversal stress (xy) seems to be uniform throughout the system. It can also be seen that the transversal stress is smaller than the longitudinal stress.

Effect of Incident energy on the characteristics of the film :

The incident energy refers to the kinetic energy of atoms or molecules as they collide or strike the substrate surface during the deposition process. If the incident energy exceeds a certain value, then the thin film deposition will not occur. In this case, the diffusion of Si atoms in the substrate is very high and also the Si atoms will bounce off the substrate and move out of the simulation box as shown in Fig 4.

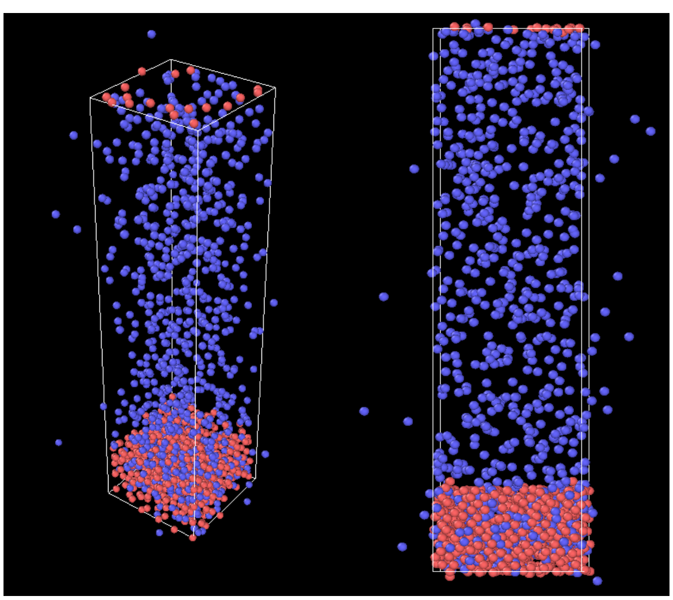


Fig 4: Images of the simulation when the incident **energy is increased by 5 times**(44.72 angstrom/ps) the initial energy

Then, we ran the thin film deposition simulation by both increasing and decreasing the Incident energy by 2 times. The following Observations were made.

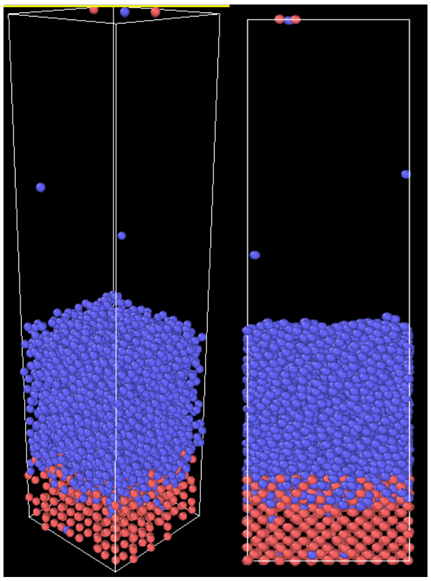


Fig 5: Incident energy **decreased by 2 times** (incident velocity = -14.14 Å/ps) the initial value

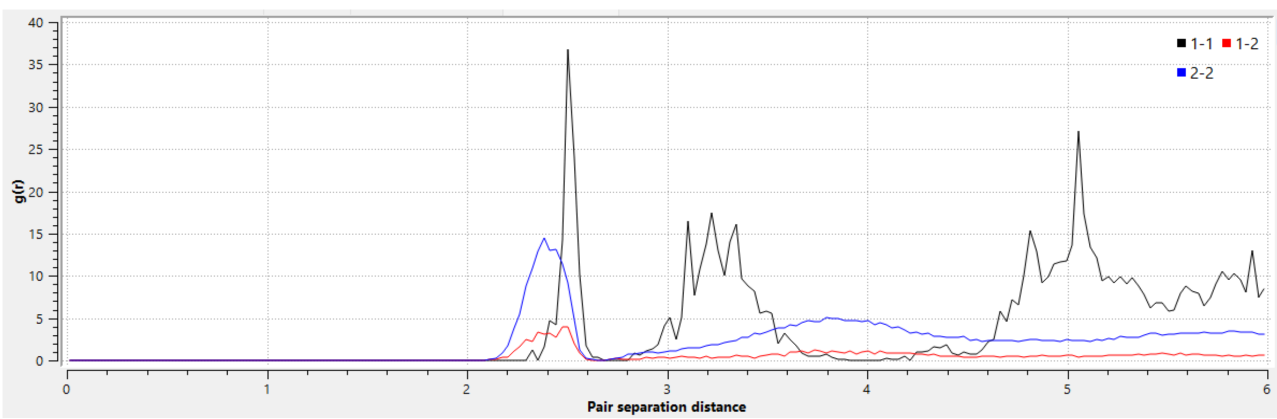


Fig 6: RDF plot for the system at Vzz =- 14.14 Å/ps

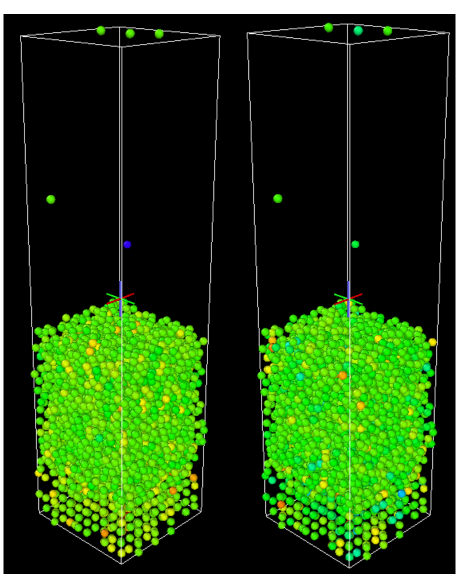


Fig 7: End simulation color coded based on (a) longitudinal (left) and (b) transversal stress (right) at incident velocity = -14.14 Å/ps

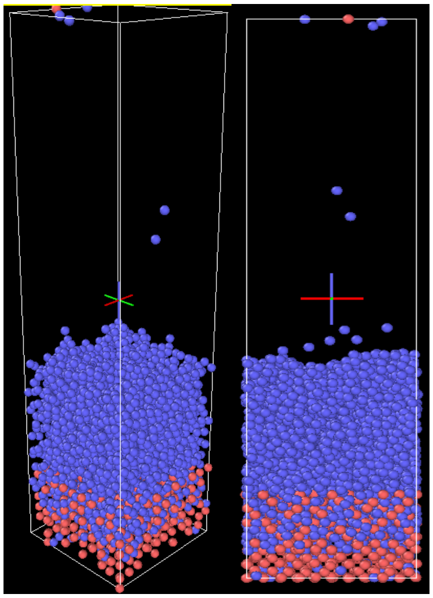


Fig 8: System at Incident velocity = -28.28 Å/ps

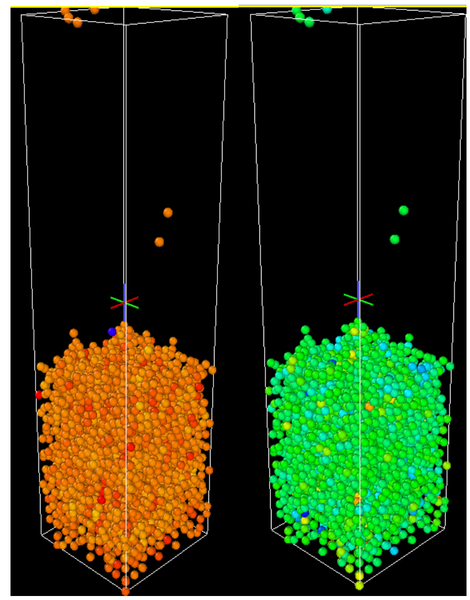


Fig 9: System color coded based on (a) longitudinal (left) and (b) transversal stress (right) Incident velocity =- 28.28 Å/ps

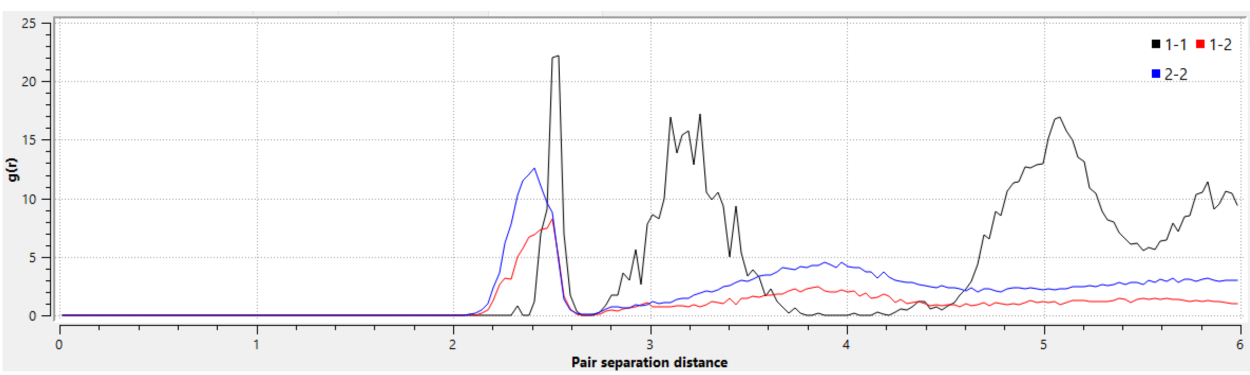


Fig 10: RDF plot for the system at Vzz = -28.28 Å/ps

From the resulting simulations, it can be said that the diffusion of Si atoms through substrates increases with increased Incident energy. The RDF plot for the depositing Si atoms remains almost the same as it is in initial conditions. At higher energies, the impinging Si atoms can displace more atoms from their equilibrium positions, introducing more defects and structural disorder in the film. This increased disorder and strain in the atomic network would result in higher intrinsic stress levels.

Effect of Substrate Temperature on the characteristics of the film :

We ran the simulation by increasing the substrate temperature to 800k and 900k.

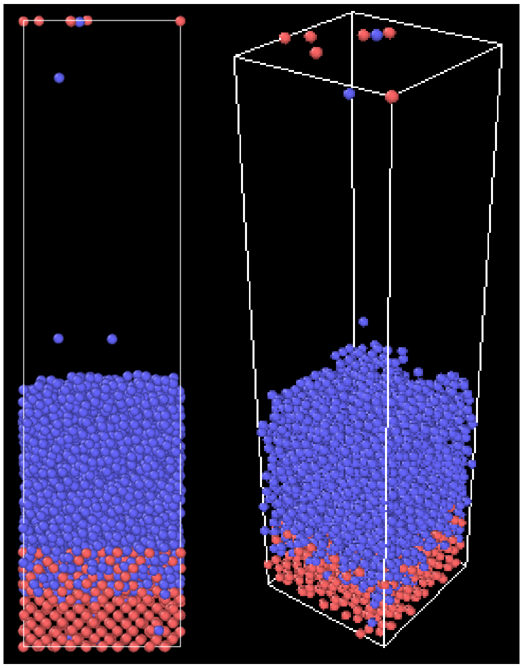


Fig 11: Thin film deposition at 800k

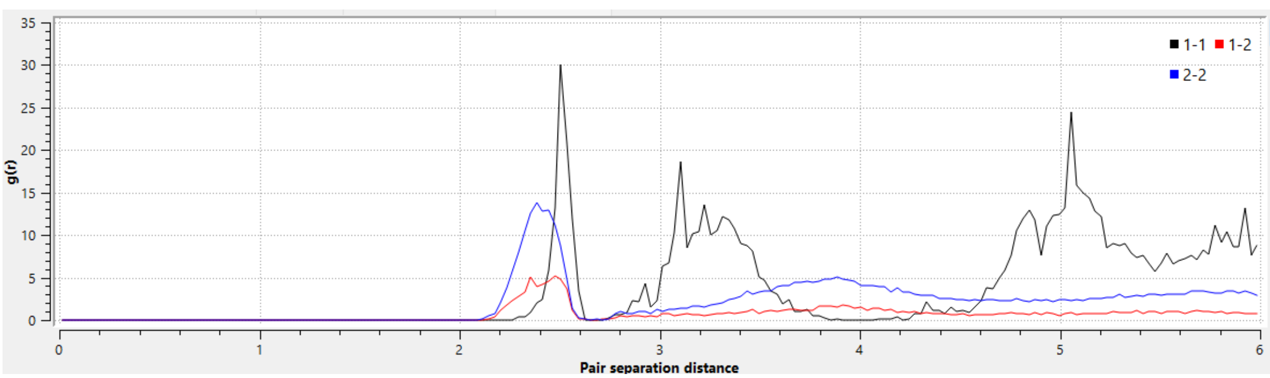


Fig 12: RDF plot for the system at 800k substrate temperature.

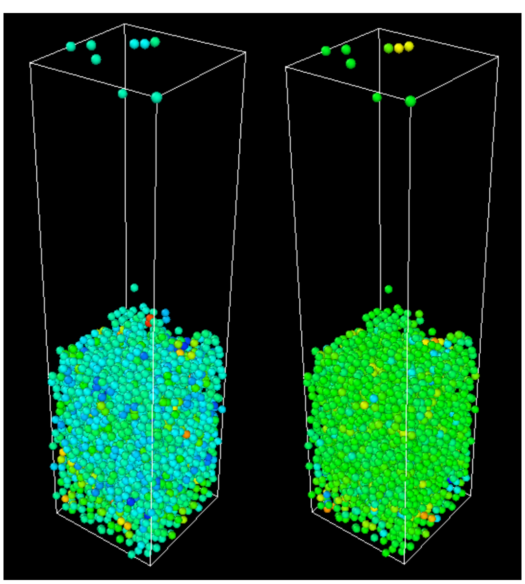
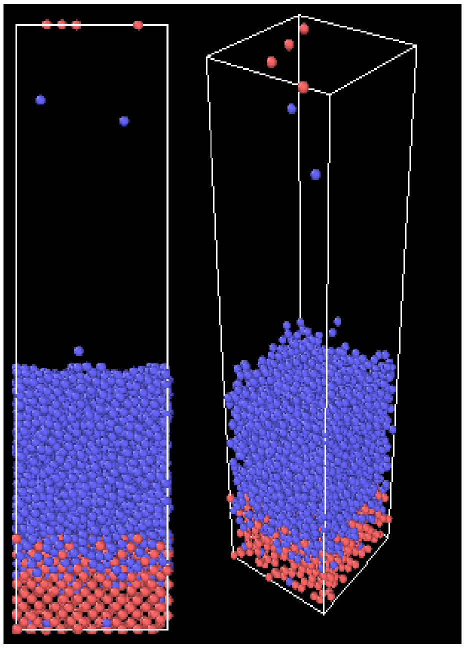


Fig 13: End simulation color coded based on (a) longitudinal stress (left) and (b) transversal stress (right) at 800k



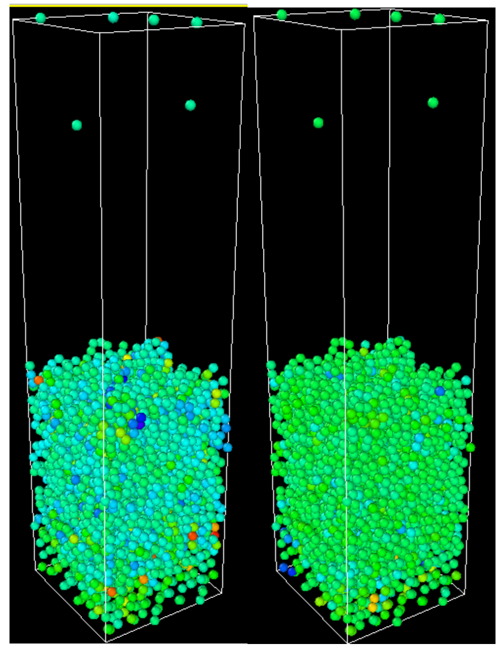


Fig 14: Thin Film deposition at 900k

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Fig 15: System color coded based on (a) longitudinal(left) and (b) transversal stress (right) at 900k

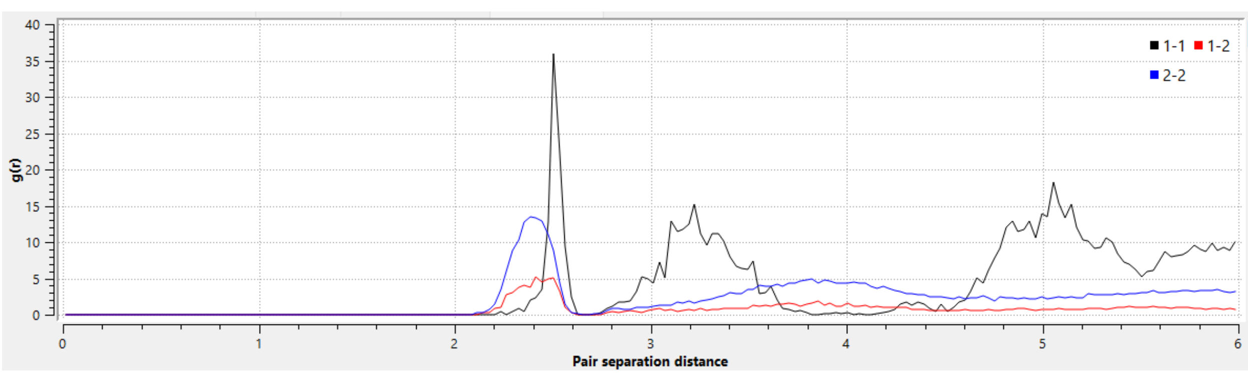

Fig 16: RDF plot at 900k

Comparing fig11 and fig14 to fig 1, it can be seen that there is not much difference in diffusion of Si atoms through substrate. It can also be observed that there is no change in the RDF plot of deposited (blue plot) atoms indicating that the characteristics of the film remain the same as it is at 300 k substrate temperature.Coming to the stress tensor, it is observed that there is decrease in longitudinal stress (zz direction) with increase in temperature as observed from fig 3, fig 13 and fig 15.Elevated temperatures provide thermal energy that allows the deposited atoms to rearrange and find lower-energy configurations, reducing the amount of structural disorder and strain in the film. This increased structural relaxation leads to lower intrinsic stress levels.

Annealing :

The system is annealed at 1000k and the stress distribution is observed. To anneal the system at 1000k, we appended the following piece of code to the input script provided to us.

```
        fix 6 film nvt temp 1000 1000 1.0
        run 100000  # for equilibration

        # to analyze the stress distribution after annealing
        compute annealed_stress all stress/atom NULL
        dump annealed_dump all custom 1000 annealed.dump id type x y z c_annealed_stress[1] c_annealed_stress[2]
c_annealed_stress[3] c_annealed_stress[4] c_annealed_stress[5] c_annealed_stress[6]
        run 100000  # Run for additional steps to analyze the stress distribution
```

Fig 17: Code that was added to the input script to anneal the system

We first heated the system till 1000k and allowed it to equilibrate. After equilibration, we computed stress tensor values and wrote the data to a file named annealed.dump

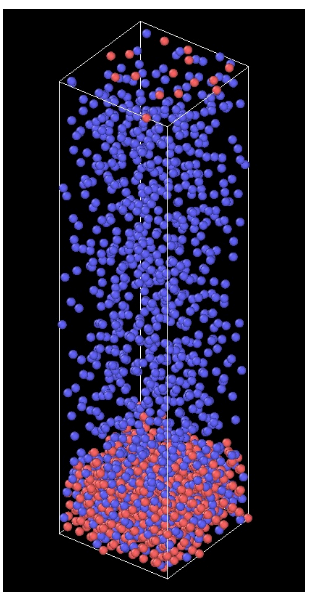

Fig 18: System after annealing is performed.

After annealing is performed, the system becomes very chaotic as the kinetic energy of the Si atoms increases due to heating.

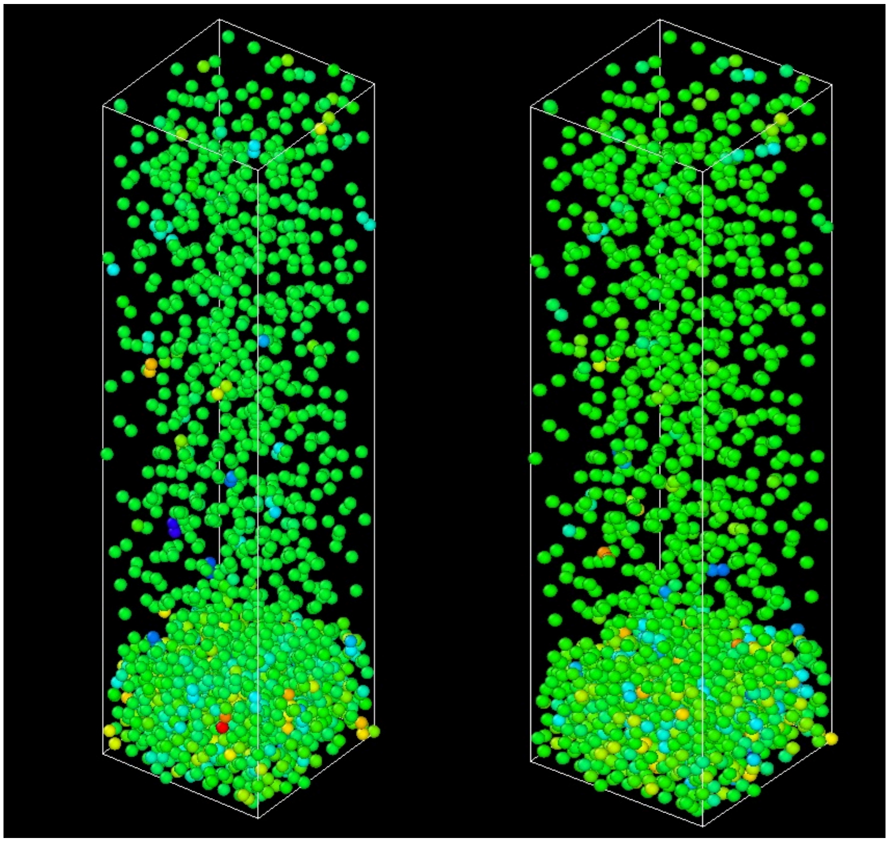

Fig 19: System color coded based on (a) longitudinal(left) and (b) transversal stress (right) after annealing the temperature at 1000k.

Annealing the a-Si film at high temperatures (e.g., 1000 K) after deposition is expected to further reduce the intrinsic stress. The high thermal energy provided during annealing allows for additional structural relaxation and defect annihilation, leading to a more ordered and less strained atomic network. This structural relaxation process would effectively relieve a significant portion of the intrinsic stress in the film.

From fig 19, it can be seen that there is a decrease in the stress as the system is annealed to 1000k. Comparing Fig 19 and Fig 13, it can be said that the effect of increasing the substrate temperature is much more on the stress than heating the deposited system to 1000 k.

Conclusion :-

In this study, we explored the thin film deposition of silicon on a crystalline silicon substrate.By characterizing the formed film through analysis of the radial distribution function (g(r)), we determined its structure to be amorphous and assessed the stresses developed within it. Additionally, we studied the effects of incident energy and substrate temperature on the film's characteristics, observing changes in structure and stress. Furthermore, annealing at a high temperature allowed us to investigate how stress distribution in the film was affected. Overall, this study provides valuable insights into the thin film deposition process of silicon on a substrate, laying the groundwork for further research and applications in semiconductor and thin film technology.

References :-

[1] Materials Science Forum Vols 449-452 (2004) pp 97-100 Online: 2004-03-15 © (2004) Trans Tech Publications, Switzerland doi:10.4028/www.scientific.net/MSF.449-452.97