Progress in Physics of Applied Materials 4 (2024) 69-76

Semnan University

Progress in Physics of Applied Materials

journal homepage: https://ppam.semnan.ac.ir/

Molecular dynamics simulation of temperature effects on the mechanical properties of Carbon polycrystalline

Maboud Hekmatifar[a], Davood Toghraie[a], Roozbeh Sabetvand [b], Shadi Esmaeili [a]*

[a] Department of Mechanical Engineering, Khomeinishahr Branch, Islamic Azad University, Khomeinishahr, Iran
[b]Department of Energy Engineering and Physics, Faculty of Condensed Matter Physics, Amirkabir University of Technology, Tehran, Iran

ARTICLE INFO

Article history:
Received: 20 January 2024
Revised: 16 March 2024
Accepted: 25 March 2024

Keywords:
Molecular Dynamics Simulation
Temperature
Mechanical Properties
Polycrystalline

ABSTRACT

The mechanical properties of carbon polycrystalline materials are crucial because they determine how the material responds to external forces, such as stress and strain, and environmental conditions. By investigating the mechanical properties of carbon polycrystalline materials, researchers can develop insights into their strength, ductility, hardness, and other characteristics, which are vital for their practical applications in industries such as manufacturing, construction, and materials science. Molecular dynamics techniques enable the examination of various polycrystalline configurations and the assessment of their effectiveness. The present study investigates the effects of temperature on the mechanical properties of Carbon polycrystalline. The results show that the ultimate strength and Young's modulus of the simulated polycrystal are 64.553 Gpa and 355.284 GPa, respectively. Also, the results showed that with increasing temperature to 320 K, Young's modulus and ultimate strength of carbon polycrystalline increase to 363.185 and 69.417 GPa, respectively. With a further increasing the temperature to 350 k, these parameters decrease to 349.909 and 63.047 GPa. The observed increase in these parameters at lower temperatures may be attributed to the increased atomic mobility of the samples resulting from the initial temperature enlargement. The simulation results are expected to help further understand the influence of temperature on the mechanical properties of carbon polycrystalline materials.

1. Introduction

A carbon polycrystal with a diamond structure comprises multiple crystalline grains of Carbon arranged in a polycrystalline structure [1, 2]. Each grain within the material has a diamond lattice structure characterized by strong covalent bonds between carbon atoms [3]. This gives the material exceptional hardness, strength, and thermal conductivity. The polycrystalline nature of the material results in grain boundaries where the crystallographic orientation of adjacent grains may differ [4, 5]. These grain boundaries can influence the material's mechanical and thermal properties, affecting deformation behavior, fracture toughness, and thermal resistance. The unique combination of properties in carbon polycrystals with a diamond structure makes them suitable for a wide range of applications, including cutting tools, abrasives, and high-temperature electronic devices [6, 7]. The material's exceptional hardness, strength, and thermal stability make it a valuable choice for demanding industrial and technological applications. Additionally, the ability to engineer the grain boundary properties allows for the customization of material behavior to suit specific requirements, further expanding the potential applications of carbon polycrystals with a diamond structure.

Various studies have been conducted on crystal and polycrystals' mechanical properties (MP). For example, Schacht et al.[8] examined the effect of empty spaces on the evolution of in crystals. According to the simulation data, voids will grow and shape in line with the crystal's orientation. Asim et al.[9] discovered that the accumulation of tiny holes made durable aluminum composite materials

---

* Corresponding author.
E-mail address: shadi.esmaeili72@yahoo.com

Cite this article as:
Hekmatifar, M., Toghraie, D., Sabetvand R. and Esmaeili, S., 2024. Molecular dynamics simulation of temperature effects on the mechanical properties of Carbon polycrystalline. *Progress in Physics of Applied Materials*, 4(1), pp.69-76.DOI: **10.22075/PPAM.2024.33046.1087**

vulnerable to breaking. Computer modeling has been used in to analyze the behavior of individual crystal aluminum alloy AAxxx5 with a range of voids and orientations. A proportion of the sample has been used to indicate the entire material. The correlation between the initial size of the space, its growth, material deformation irregularities, and the effect of small-scale size has been established. Liu et al.[10] using a model that accounts for time difference, investigated the behavior of crystals and biocrystals with different levels of gaps in response to small-scale tension changes. It has been found that the change in approach, configuration of vacant spaces, and application of pressure exert a major influence on Al's power. While investigating polycrystalline crystals, Si [11] used an automatic computer program that simulated homogeneous aluminum deformation when squeezed. They have tested the program to verify that it is working properly. It would, therefore, appear that the approach is appropriate for application. Working with A1-Zn-Mg alloy single crystals, Wilhelm [12] found a flat area in the CSSC. Lee et al.[13] examined the durability of an A1-Cu alloy metal. As they have discovered, this metal's single-crystal and polycrystal forms exhibit comparable strength. To see if the similarity between mono and polycrystalline A1Cu alloy behavior also applies to ternary AIZn+Mg alloys, this study compared results from a polycrystalline alloy with Wilhelm's work.

A carbon polycrystal with a unique structure exhibits distinctive MP characterized by a complex deformation behavior and exceptional thermal resistance. The material's non-uniform grain boundaries and crystallographic orientations contribute to its diverse mechanical response. These features make it an intriguing subject for research on material behavior and its application in high-stress environments. This study investigates the influence of temperature on the MP of carbon polycrystals through molecular dynamics (MD) simulations. By analyzing stress-strain curves, ultimate strength (US), and Young's modulus (YM) at different temperatures (300 K, 310 K, 320 K, and 350 K), the research aims to enhance the understanding of material behavior and facilitate advancements in material science, engineering design, and product development.

The novelty of this study in utilizing MD simulation to assess the impact of temperature on the mechanical properties of carbon polycrystals stems from its capability to offer unparalleled atomic-scale granularity. Through intricate modeling of the dynamic interactions among atoms ensconced within the crystal lattice, MD simulations afford an exhaustive comprehension of the multifaceted ways temperature influences material behavior. This encompasses a broad spectrum of mechanical attributes, encompassing not only elasticity but also strength, fracture toughness, and beyond, thereby presenting a comprehensive depiction of the material's response to varying thermal environments. This research endeavor is geared towards unraveling the intricate interplay between temperature variations and the mechanical responses of carbon polycrystals, thereby fostering the development of predictive models capable of elucidating material behaviors across a gamut of thermal scenarios. By leveraging this innovative approach, a deeper comprehension of carbon polycrystals' mechanical attributes is cultivated, paving the way for informed material design strategies tailored to meet the exacting demands of specific engineering applications.

2. Molecular dynamics simulation

According to the laws of physics, MD is based on computer simulations to replicate particle behavior. It helps to clarify how the motion of particles is understood [14]. MD simulation is used to investigate how particles move in a system. Such an approach is to solve the Newton equations for each particle in a system by itself [15]. This allows for the early prediction of all particles' movements at a given time. The MD simulation is a computational technique used in various scientific disciplines to gain insight into the dynamics and properties of complex systems at the atomic and molecular scale. The LAMMPS software was used for comprehensive simulations based on Newton's second law, which describes the relationship between force, acceleration, and particle mass [16, 17]:

$$F_i = \sum_{i \neq j} F_{ij} = m_i \frac{d^2 r_i}{dt^2} = m_i \frac{dv_i}{dt} \tag{1}$$

On the other hand, F_i is obtained from the negative derivative of the potential function U [16]:

$$F_i = -\nabla U_i = -\frac{\partial U}{\partial r_i} \tag{2}$$

The first step in the MD simulation is to define the system, including specifying particles, initial position and velocity, and any constraints or boundary conditions. A force field is then used to describe particle interactions within the system. It includes terms for bonding interactions (such as covalent bonds), nonbonding interactions (such as van der Waals forces electrostatic interactions), and other potential energy terms. The total interactions among particles in the system determine the overall energy level of the system [18, 19].

$$E_{total} = E_{bonded} + E_{nonbonded} \tag{3}$$

Different energy forms arise as a result of the interaction between atoms. The current research uses the Tersoff potential function to determine the interactions between carbon atoms in the simulation system. The mathematical relationship describing the Tersoff potential function is as follows [20]:

$$E = \frac{1}{2} \sum_{i} \sum_{j \neq i} U_{ij} \tag{4}$$

$$U_{ij} = f_C(r_{ij})\left[a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \tag{5}$$

$$f_C(r) = \begin{cases} 1 & r < R - D \\ \frac{1}{2} - \frac{1}{2} sin(\frac{\pi}{2} \frac{r - R}{D}) & R - D < r < R + D \\ 0 & r > R + D \end{cases} \tag{6}$$

In Eq. (8), f_R is the absorbent particle interaction with the general form as follows:

$$f_R(r) = A\, exp(-\lambda_1 r) \tag{7}$$

and f_A is the particle-repellent interaction with the general form as follows:

$$f_A(r) = -B\, exp(-\lambda_2 r) \tag{8}$$

In the above equations, A, B, and λ are the potential constants and depend on the studied structures. b_{ij} defined in (8) equation is determined as follows:

$$b_{ij} = \left(1 + \beta^n {\varphi_{ij}}^n\right)^{-\frac{1}{2n}} \tag{9}$$

$$\varphi_{ij} = \sum_{k\neq ij} f_C(r_{ik}) g(\theta_{ijk}) exp[\lambda_3^m (r_{ij} - r_{ik})^m] \tag{10}$$

The function of g(θ) is related to the angle between i and j particles and between i and k particles.

2.1. Present simulation details

In this study, a computer model is applied to determine the MP of Carbon polycrystalline by looking at the effects of initial temperature using LAMMPS software [21]. AtomSK software was used to model a representation of the Carbon polycrystalline [22]. Next, we use the NVE ensembles to minimize this process with more than 100,000 steps. Minimization is a method of computing in which the atoms' and molecules' positions are repeated to reduce potential energy so that we can detect the lowest state of the system. It will help to achieve a more stable, energy-efficient configuration of the simulation system. Next, the temperature and pressure are set in the NPT ensemble at 300 K and 1 bar, respectively, using an equilibration process. The equilibration of the simulated structure was checked during 200,000-time steps by the change in the temperature and potential energy. Figure 1 represents the schematic of the carbon polycrystalline structure. The simulation details implemented in the current MD research are outlined in Table 1.

3. Equilibration Process

Fig. 2 represents the temperature change in simulated atomic samples during 2100,000 time steps. The simulation results indicate that the system's temperature converged to 300 K after 200,000 time steps. This convergence suggests that the simulated system reached a stable thermal equilibrium at 300 K, indicating the simulation's effectiveness in capturing the Carbon polycrystalline material's thermodynamic behavior.

Table 1. The MD simulation parameters in the simulated structure.

MD Simulation Setting	Value or Method
MD Box Length(A)	50×50×50 Å^3
Number of Atoms	22044
Boundary Condition	p p p
Initial Temperature	300 K
Initial pressure	1 bar
Thermostat	Nose-Hoover
Time Step	1 fs

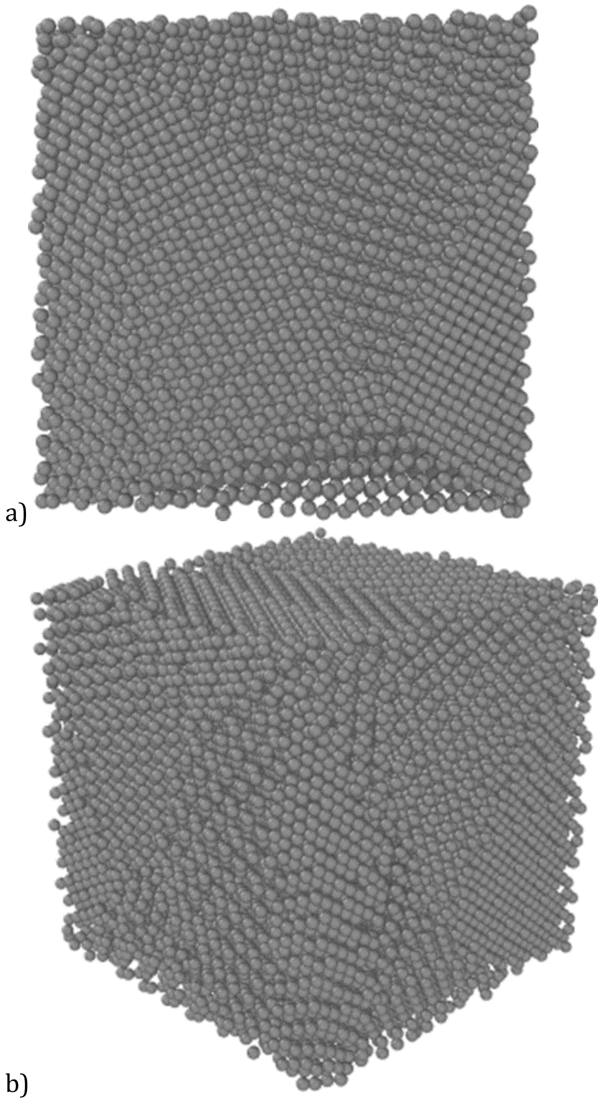

Fig.1 A schematic of carbon polycrystalline structure from a) side and b) perspective view.

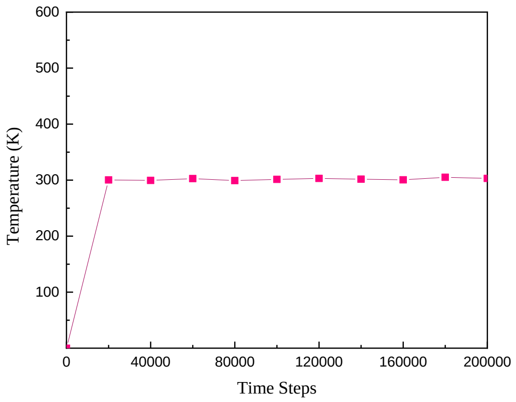

Fig. 2. The temperature change in simulated atomic samples during 200,000 time steps.

Fig. 3 represents the changes in the potential energy of carbon polycrystalline during 200,000 time steps. The data revealed that as the simulation progressed, the system's potential energy reached a stable value of -6.87 eV, indicating that the system had achieved equilibrium in terms of potential energy. This convergence of potential energy is an important indicator of the stability and thermodynamic equilibrium of the simulated carbon polycrystalline material. The negative value of the potential energy indicates an attractive force between the particles in the carbon polycrystalline system. The convergence of the potential energy to a stable value of -6.87 eV signifies that the force field used in the simulation is appropriate, and the simulation has been run for a sufficient duration to reach a state of equilibrium where the system's potential energy has stabilized. This indicates that the simulation captures the suitable interactions and dynamics of the carbon polycrystalline material. These results are in good agreement with previous results. [21-23]

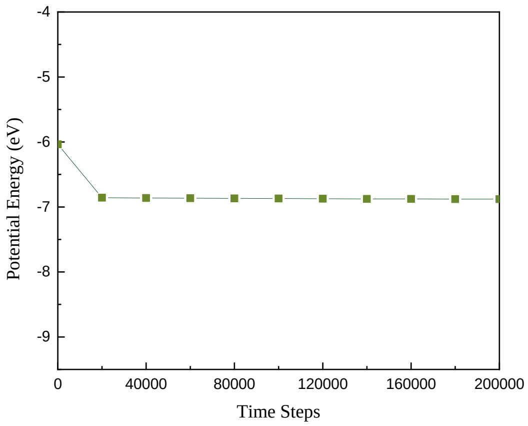

Fig. 3. The potential energy change in simulated atomic samples during 100,000 time steps.

4. Validation

The radial distribution function (RDF) is important in molecular dynamics simulations because it provides valuable information about particle spatial arrangement and organization in a system. By analyzing the RDF, researchers can gain insights into the structure, density, and interactions between particles, which are crucial for understanding the thermodynamics and MP of the simulated material. The RDF helps characterize the local environment around a particle, identifying the presence of ordering and studying the distribution of particles within the simulation system. Overall, the RDF is a powerful tool for investigating materials' structural properties and behavior at the atomic and molecular level in molecular dynamics simulations. Figure 4 represents the RDF of carbon particles in the present study, which agrees with previous papers [24].

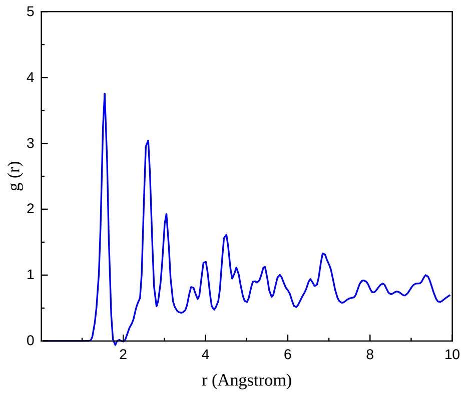

Fig.4. The RDF of carbon particles in the present study.

5. Results and discussion

After reaching equilibrium, the carbon polycrystalline was subjected to tensile loading along the X-axis with a magnitude of 1 s^{-1} from both sides by increasing the initial temperature from 300 to 350 K to investigate the simulated structure's MP. Figure 5 illustrates a schematic of the mechanical test of the carbon polycrystalline. Consequently, the strain stress, US, and YM diagrams were examined.

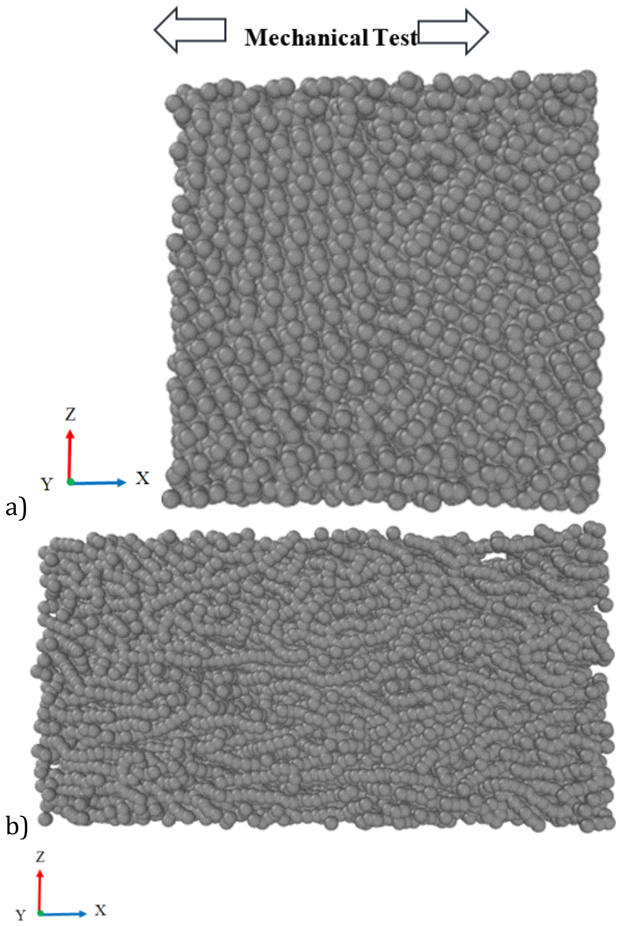

Fig. 5. A schematic of equilibrated carbon polycrystalline structure a) before and b) after tensile test.

Fig. 6 shows the stress-strain curve of simulated carbon polycrystalline. The two peaks in the strain-stress curve of a carbon polycrystalline with a diamond structure are due to the different deformation mechanisms that occur at different stress levels. The first peak represents the onset of plastic deformation, where dislocations start to move, and the material undergoes irreversible deformation. The second peak corresponds to the failure of the material, where cracks propagate and lead to catastrophic failure. The presence of two distinct peaks in the strain-stress curve reflects the complex behavior of the material under stress, taking into account both plastic deformation and ultimate failure. The YM is typically calculated from the initial linear portion of the stress-strain curve, which corresponds to the elastic region. This is usually the portion of the curve before the onset of plastic deformation, and it is associated with the first peak in the stress-strain curve. Conversely, the US is determined from the maximum stress value on the stress-strain curve, which corresponds to the second peak in the curve. This peak represents the maximum stress the material can withstand before failure occurs. The results show that the US and YM of simulated polycrystal are 64.553 Gpa and 355.284 GPa, respectively. In the previous papers, Wei et al. [25] conducted an examination focusing on the mechanical characteristics of a carbon nanostructures. They found that the US of this structure falls within the range of 60 to 80 GPa, indicating its robustness under various mechanical stresses. In a similar study, Xu et al. [26] investigated the mechanical properties of polycrystalline graphene oxide. Through detailed simulations, they observed changes in the ultimate stress values in the material, which with increasing temperature from 100 to 1250 K, the ultimate strength levels between 30 and 40 GPa was fluctuating. These findings emphasize the complex interplay between temperature and mechanical properties in polycrystalline graphene oxide and emphasize the importance of understanding such dynamics for engineering applications.

The initial temperature can affect the atomic evolution of carbon polycrystalline. This evolution changes their mechanical performance, causing various parameters such as US and YM to converge to different values. It is worth to mention that the increase of parameters such as US and YM in polycrystalline carbon due to initial temperature changes can be explained by the interplay between thermal expansion effects, material properties, and atomic-level processes. Elevated temperatures increase atomic vibrations, causing thermal expansion and reducing YM. This expansion induces internal stresses, but as temperature rises further, the rate of thermal expansion decreases, and the reduction in modulus stabilizes due to a balance between thermal energy and material stiffness. Within this convergence range, critical temperatures facilitate atomic diffusion, defect formation, and influencing the material's atomic evolution. Figure 7 illustrates that the mechanical strength of the carbon polycrystalline improved as the temperature increased to 320 K. With further increasing temperature to 350 K, this mechanical strength decreased. This change in mechanical performance is attributed to the decreasing attraction force between carbon polycrystalline particles. From an atomistic perspective, the increase in temperature leads to higher atomic mobility of carbon atoms through the $1/2mv^2=3/2kT$ relation, so the attraction force between polycrystalline carbon particles decreases. This weakening of the inter-particle attraction results in a reduction in the mechanical strength of the material.

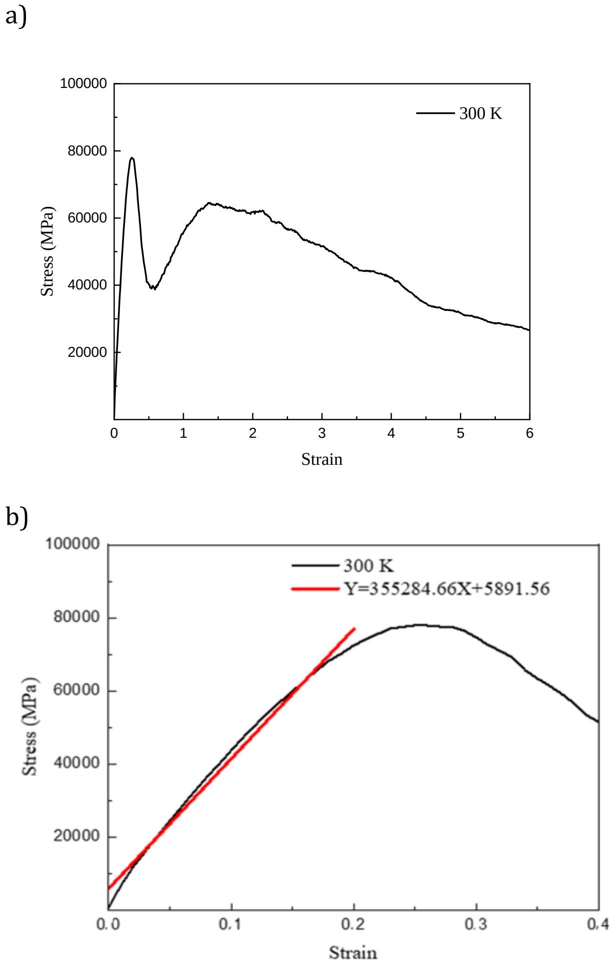

Fig.6. The a) stress-strain curve and b) Young's modulus of Carbon polycrystalline at 300 K.

Fig. 8 and 9 represent the change in US and YM of carbon polycrystalline at different temperatures. The results showed that increasing temperature to 320 K, the YM and US of carbon polycrystalline increase to 363.185 and 69.417 GPa. With a further increase to 350 k, these parameters decrease to 349.909 and 63.047 GPa. The observed increase in these parameters at lower temperatures may be attributed to the increased atomic mobility of the samples resulting from the initial temperature enlargement. Also, the material's thermal expansion at lower temperatures may reduce internal stresses, increasing the YM and ultimate strength. However, as the temperature rises, thermal expansion may dominate, causing a decrease in these parameters. The increase in temperature can lead to enhanced mobility of grain boundaries within the polycrystalline structure. This increased mobility may initially contribute to improved MP. However, excessive grain boundary mobility can reduce the material's mechanical strength at higher temperatures.

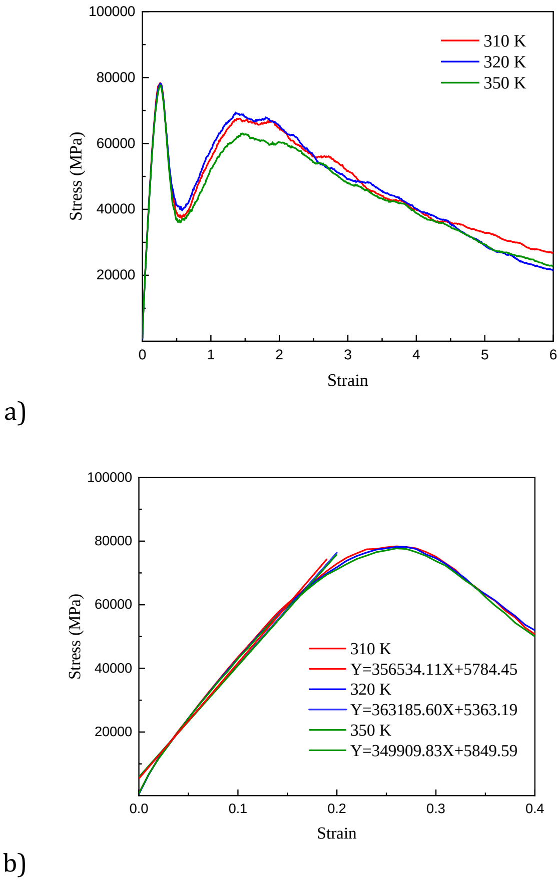

Fig.7. The a) stress-strain curve and b) YM of Carbon polycrystalline at different temperatures.

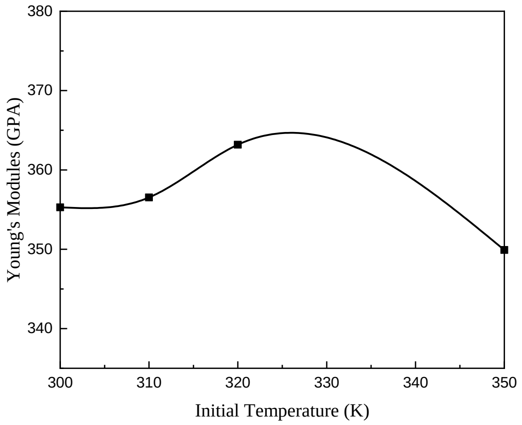

Fig. 8. The YM variation of the Carbon polycrystalline with increasing initial temperatures.

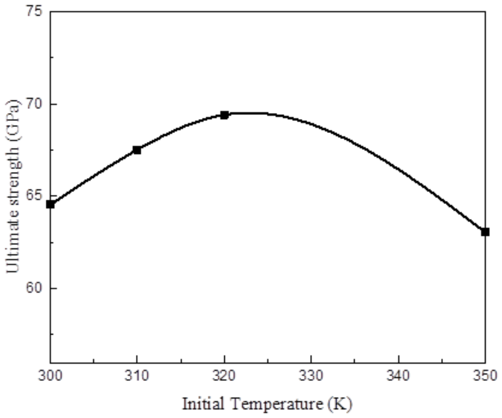

Fig. 9. The US variation of the Carbon polycrystalline with increasing initial temperatures.

Table 2. The change in the US and Young's Modules of Carbon polycrystalline at different temperatures.

Initial Temperature (K)	**Young's Modules (GPA)**	US **(GPa)**	
		First Peak	**Second Peak**
300	355.284	77.963	64.553
310	356.534	78.172	67.527
320	363.185	78.351	69.417
350	349.909	77.704	63.047

6. Conclusion

In conclusion, the molecular dynamics simulation in the present study has provided valuable insights into the effects of temperature on the MP of carbon polycrystalline materials. The observed changes in the US and YM with increasing temperature have highlighted the significant influence of thermal conditions on the material's mechanical behavior. These findings are crucial for understanding the performance of carbon polycrystalline materials in real-world applications, such as manufacturing and construction. They can contribute to developing more accurate predictive models for material behavior under varying thermal environments. The numerical results are summarized as follows:

- The simulation results indicate that the system's temperature converged to 300 K after 200,000 time steps. This convergence suggests that the simulated system reached a stable thermal equilibrium at 300 K, indicating the simulation's effectiveness in capturing the carbon polycrystalline material's thermodynamic behavior.
- The results revealed that as the simulation progressed, the system's potential energy reached a stable value of -6.87 eV, indicating that the

system had achieved equilibrium in terms of potential energy.

- The results show that the US and YM of simulated polycrystal are 64.553 Gpa and 355.284 GPa, respectively.
- The results showed that increasing temperature to 320 K, YM, and US of carbon polycrystalline increase to 363.185 and 69.417 GPa. With a further increase to 350 k, these parameters decrease to 349.909 and 63.047 GPa. The increase in temperature can lead to enhanced mobility of grain boundaries within the polycrystalline structure. This increased mobility may initially contribute to improved MP. However, excessive grain boundary mobility can reduce the material's mechanical strength at higher temperatures.

Acknowledgements

There is nothing to acknowledgement.

Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this article.

References

[1] Shenderova, O.A. and McGuire, G., 2006. Types of nanocrystalline diamond. In *Ultrananocrystalline diamond* (pp. 79-114). William Andrew Publishing.

[2] De, S., Heaney, P.J., Fei, Y. and Vicenzi, E.P., 2004. Microstructural study of synthetic sintered diamond and comparison with carbonado, a natural polycrystalline diamond. *American Mineralogist*, *89*(2-3), pp.438-446.

[3] Field, J.E., 2012. The mechanical and strength properties of diamond. *Reports on Progress in Physics*, *75*(12), p.126505.

[4] Hansen, N., Huang, X. and Winther, G., 2011. Effect of grain boundaries and grain orientation on structure and properties. *Metallurgical and Materials Transactions A*, *42*, pp.613-625.

[5] Van Der Zande, A.M., Huang, P.Y., Chenet, D.A., Berkelbach, T.C., You, Y., Lee, G.H., Heinz, T.F., Reichman, D.R., Muller, D.A. and Hone, J.C., 2013. Grains and grain boundaries in highly crystalline monolayer molybdenum disulphide. *Nature materials*, *12*(6), pp.554-561.

[6] Li, G., Rahim, M.Z., Pan, W., Wen, C. and Ding, S., 2020. The manufacturing and the application of polycrystalline diamond tools–A comprehensive review. *Journal of Manufacturing Processes*, *56*, pp.400-416.

[7] Zhang, J., Wang, J., Zhang, G., Huo, Z., Huang, Z. and Wu, L., 2023. A review of diamond synthesis, modification technology, and cutting tool application in ultra-precision machining. *Materials & Design*, p.112577.

[8] Schacht, T., Untermann, N. and Steck, E., 2003. The influence of crystallographic orientation on the deformation behaviour of single crystals containing microvoids. *International Journal of Plasticity*, *19*(10), pp.1605-1626.

[9] Asim, U., Siddiq, M.A. and Demiral, M., 2017. Void growth in high strength aluminium alloy single crystals: a CPFEM based study. *Modelling and Simulation in Materials Science and Engineering*, *25*(3), p.035010.

[10] Liu, L.Y., Yang, Q.S. and Zhang, Y.X., 2019. Plastic damage of additive manufactured aluminium with void defects. *Mechanics Research Communications*, *95*, pp.45-51.

[11] Si, L.Y., 2009. Simulation of the texture evolution during cold deformation of FCC metal with crystal plasticity FEM. *Northeastern University, China*.

[12] Wilhelm, M., 1981. The cyclic stress-strain behaviour of age-hardened Cu⍰ Co and Al⍰ Zn⍰ Mg alloy single crystals. *Materials Science and Engineering*, *48*(1), pp.91-106.

[13] Horibe, S., Lee, J.K. and Laird, C., 1984. CYCLIC DEFORMATION OF A1-4% Cu ALLOY POLYCRYSTALS CONTAINING θ ″PRECIPITATES: GRAIN SIZE DEPENDENCE AND CORRELATION WITH MONOCRYSTALLINE CYCLIC DEFORMATION. *Fatigue & Fracture of Engineering Materials & Structures*, *7*(2), pp.145-154.

[14] Van Gunsteren, W.F. and Berendsen, H.J., 1990. Computer simulation of molecular dynamics: methodology, applications, and perspectives in chemistry. *Angewandte Chemie International Edition in English*, *29*(9), pp.992-1023.

[15] Zhu, H.P., Zhou, Z.Y., Yang, R.Y. and Yu, A.B., 2007. Discrete particle simulation of particulate systems: theoretical developments. *Chemical engineering science*, *62*(13), pp.3378-3396.

[16] Rapaport, D.C., 2004. *The art of molecular dynamics simulation*. Cambridge university press.

[17] Rapaport, D.C., 2004. *The art of molecular dynamics simulation*. Cambridge university press.

[18] Nordholm, S. and Bacskay, G.B., 2020. The basics of covalent bonding in terms of energy and dynamics. *Molecules*, *25*(11), p.2667.

[19] Jiao, L., Zhu, J., Zhang, Y., Yang, W., Zhou, S., Li, A., Xie, C., Zheng, X., Zhou, W., Yu, S.H. and Jiang, H.L., 2021. Non-bonding interaction of neighboring Fe and Ni single-atom pairs on MOF-derived N-doped carbon for enhanced CO2 electroreduction. *Journal of the American Chemical Society*, *143*(46), pp.19417-19424.

[20] Tersoff, J., 1988. New empirical approach for the structure and energy of covalent systems. *Physical review B*, *37*(12), p.6991.

[21] Jiang, Y., Dehghan, S., Karimipour, A., Toghraie, D., Li, Z. and Tlili, I., 2020. Effect of copper nanoparticles on thermal behavior of water flow in a zig-zag nanochannel using molecular dynamics simulation. *International Communications in Heat and Mass Transfer*, *116*, p.104652.

[22] Jin, K., Tai, Y., Toghraie, D. and Hekmatifar, M., 2022. The effects of nanoparticle percentages and an external variable magnetic field on the atomic and thermal behaviors in an oscillating heat pipe via molecular dynamics simulation. *Journal of Molecular Liquids*, *360*, p.119570.

[23] Liu, X., Patra, I., Kuzichkin, O.R., Zaidi, M., Abdulnabi, S.M., Najm, Z.M., Altimari, U.S., Hadrawi, S.K., Andani, M.T. and Hekmatifar, M., 2022. Molecular dynamics study of the

effect of external electric field amplitude and cavity on thermal properties of Ammonia/Copper Nano-Refrigerant. *Journal of Molecular Liquids*, *365*, p.120125.

[24] Hirai, H., Terauchi, M., Tanaka, M. and Kondo, K., 1999. Band gap of essentially fourfold-coordinated amorphous diamond synthesized from C 60 fullerene. *Physical review B*, *60*(9), p.6357.

[25] Wei, Q., Zhang, Q., Yan, H. and Zhang, M., 2017. A new superhard carbon allotrope: Tetragonal C 64. *Journal of Materials Science*, *52*, pp.2385-2391.

[26] Xu, X., Xiong, C., Mao, S. and Yao, W., 2022. Established Model on Polycrystalline Graphene Oxide and Analysis of Mechanical Characteristic. *Crystals*, *12*(3), p.382.