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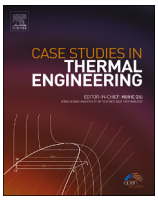

Effect of temperature on the mechanical properties of aluminum polycrystal using molecular dynamics simulation

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ABSTRACT

The initial temperature has a considerable effect on aluminum polycrystals' physical stability and mechanical performance, with the possibility to optimize their mechanical properties for practical applications. Thus, using a molecular dynamics technique, the effect of temperature on the mechanical properties of aluminum polycrystals is studied. Stress-strain curves, ultimate strength, and Young's modulus were all measured at temperatures of 300, 350, 400, and 450 K. The findings from MD simulations show that the initial temperature significantly affects the physical stability and mechanical performance of designed aluminum polycrystals. The aluminum polycrystal experiences a numerical increase in ultimate strength and Young's modulus from 6640 to 74.072 to 7.055 and 79.226 GPa, respectively, when subjected to the optimal initial conditions of 350 K. With further increasing temperature to 450 K, ultimate strength and Young's modulus decrease to 6.461 and 74.413 GPa, respectively. The observed decrease in ultimate strength and Young's modulus of the aluminum polycrystal as the temperature increased from the optimal condition of 350 K–450 K can be attributed to the weakening of interatomic attraction forces at higher temperatures. This reduction in interatomic bonding strength resulted in decreased material stiffness and resistance to deformation, leading to lower ultimate strength and Young's modulus values. This study's novelty lies in its comprehensive assessment of the initial temperature's effects on the mechanical performance of aluminum polycrystals, providing valuable insights for practical applications and advancing beyond previous efforts in the literature.

1. Introduction

Polycrystals are structures in which atoms, molecules, and ions coordinate on a geometric grid that shapes their boundaries [1]. High melting and boiling points are the properties of ion and metallic polycrystals. Using techniques, such as molecular dynamics

Abbreviations: Al, Alumunium; MD, Molecular dynamics; Cu, Copper; US, ultimate strength; YM, Young's modules.

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(MD), it can generate accurate atomic models and observe the physical and chemical properties of these polycrystalline structures [2]. Based on where testing occurs, crystalline solids may show differences in strength. This product may be applied to the manufacturing of materials with several crystals. The complexity of crystals' shapes and angles continues to grow more complex; not all solutions are possible with testing or computer simulations [3]. Polycrystals can increase their strength by exploiting the features of nanoparticles and edges using different combinations of materials [4,5]. Adjustments to the system for each material may be carried out to improve efficiency. In general, given the number of factors that need to be considered, simulations or trials can become excessively costly and complex. Traditional composite production methods by experimentation and simulation of solid particles are not effective enough to find new materials [6–9]. Alumunium (Al) alloy is widely used because of its strength, durability and environmental benefits. In aircraft and high speed trains, they are used because of these properties [10]. Conversely, comprehending the effect of temperature on the mechanical properties of polycrystalline materials is crucial due to its direct correlation with the performance and behavior of the materials in practical contexts. Temperature changes have the potential to greatly influence the strength, rigidity, ductility, and resistance to deformation of a material. These properties are pivotal in assessing the material's appropriateness for particular engineering and manufacturing purposes. By comprehensively studying the effect of temperature, engineers and researchers can optimize material performance, enhance durability, and ensure reliable operation under different thermal conditions, ultimately leading to the development of more resilient and efficient materials for a wide range of industries, such as aerospace, automotive, construction, and electronics.

In general, various factors, such as porosity, cavity, tension, initial temperature, etc. Can affect the mechanical properties of crystal/polycrystals. For instance, Wu et al. [11] examined the effect of temperature at mechanical propertice of cube crystal. The results reveal that in some cases, the mechanical strength of crystals increases strongly with changing temperature, while others exhibit very weak temperature dependencies. Shahshahani et al. [12] focused on the temperature effect on the mechanical propertice of porous hydrogels. The results demonstrate that the mechanical properties of hydrogel were affected by the initial temperature. Liu et al. [13] analyzed how crystals and biocrystals respond to minor tension changes with various gap levels, incorporating time differences into his model. Modifying procedures, organizing vacant areas, and exerting force on them can strengthen Al. Asim et al. [14] discovered that numerous tiny holes were why durable aluminum materials broke so easily. Computer models were utilized to analyze the behavior of individual pieces of a specific type of aluminum alloy A. A relationship was discovered between the initial size of the space, its subsequent growth, material alterations, and the effect of small size. Schacht et al. [15] developed a make-believe computer simulation to analyze the transformation of empty spaces within crystals over time. According to the simulation, empty spaces will expand and alter their form in alignment with the crystal's orientation. Wilhelm [16] examined the cyclic hardening and softening of specific alloys at different strain amplitudes, emphasizing the formation of persistent slip bands and discussing their limited strain capacity. In contrast to single-phase alloys and pure metals, the results indicate that analogous behavior could be anticipated from additional age-hardened substances. Lee et al. [17] conducted a test to determine the strength of the A1-copper (Cu) alloy metal. Compared to another study focusing on the behavior of A1Cu, particularly when combined with other metals, it found similar results. Mahjoory et al. [18] focused on the mechanical properties of calciumphosphate. The inclusion of nanoparticles enhances the mechanical properties of modeled structure, as demonstrated by the results. Fada et al. [19] focused on the mechanical properties of calciumphosphate. The results indicate that the changes in the mechanical properties of the simulated structures were caused by variations in porosity.

Previous studies showed that the mechanical strength of polycrystalline materials can be affected by temperature changes via several mechanisms. At elevated temperatures, the thermal energy may enhance the movement of dislocations inside the material, resulting in a decrease in its strength. In addition, temperature changes may affect the microstructure, grain boundaries, and atomic interactions of a material, hence affecting its mechanical properties. This study aimed to investigate the effect of temperature on the mechanical properties of aluminum polycrystalline using MD simulation. The stress-strain curves, ultimate strength (US), and Young's modulus (YM) were calculated at temperatures of 300, 350, 400, and 450 K. This approach provided valuable insights into the temperature-dependent behavior of the material, offering a deeper understanding of its mechanical response across a range of thermal conditions. Finally, the results of this study led to improvements in material science, engineering design, production methods, and product development resulting in a higher degree of performance and reliability.

2. Methodology

In this experiment, the MD approach was used to model the temporal behavior of atoms and molecules, enabling the examination of the mechanical properties of aluminum polycrystals at various temperatures. This approach offers a comprehensive comprehension of the atomic-level behavior of the material, providing valuable insights on its mechanical properties under different circumstances. It is due to the MD simulates the motion of atoms and molecules over time, considering their interactions and behavior at the atomic level [20,21]. Through the monitoring of the coordinates and velocities of solitary particles, MD enables the examination of the material's thermal response, thereby furnishing precise and comprehensive information regarding its mechanical properties. MD simulation is employed to examine the group dynamics of particles. This technique resolves Newton's equations for each separate particle within a system [22]. This is used to anticipate the specific whereabouts of all particles at a certain time. Investigate how various particles behave and interact in MD simulations. Potential function has two capabilities: bounded and unbounded. How the particles interact with each other, bonded or not, is a determining factor in the energy level of the system [23,24].

$$E_{total} = E_{bonded} + E_{nonbonded} \tag{1}$$

The interaction of atoms leads to the generation of different forms of energy. Using Lennard Jones' potential, it can gauge the total energy by analyzing the values of a function [25,26]. EAM Potential function was utilized to analyze the interaction among metal particles using a specific mathematical formula [27].

$$U_i = F_\alpha \left(\sum_{i \neq j} \rho_\beta \left(r_{ij} \right) \right) + \frac{1}{2} \sum_{i \neq j} \varphi_{\beta\alpha} \left(r_{ij} \right) \tag{2}$$

In Eq. (2), φ_β represents the repulsive force, ρ_β represents the attractive force, and r_{ij} are the distance of particles from each other.

2.1. Simulation details

Present study investigates the effect of temperature on the mechanical properties of aluminum polycrystal using MD simulation. First, AtomSK software [28] was utilized to Al polycrystalline structure with the dimention of 50 Å in all directions (See Fig. 1). Next, using LAMMPS software [29], the initial modling structure is simulated with definding EAM force filed. The periodic boundary condition periodic was set. Next, for ensuring the sutable setting, the equilibration was checked during 100,000 time-steps. In this stage, the NPT ensemble is used. At 300 K and 1 bar, the NPT ensemble regulates temperature and pressure via minimization. NPT ensembles are utilized in simulations to replicate variables including temperature, pressure, and particle quantity. In order to enhance the realism of the system's behavior, this methodology evaluates various circumstances. The time step was set 1 fs. The choice of a 1 fs time step in the present simulation was considered appropriate based on the specific dynamics of the system being studied. In the context of an MD simulation, the equilibration process can provide insight into the suitability of chosen time step by assessing whether the system reached a thermodynamically consistent state within the specified time scale. After ensuring the equilibration of modeled structures, the strength of simulated polycrystals was tested by stretching them from one side to the other with a specific force. The mechanical properticee of structure was checked with the change in the US and YM of structure.

2.2. The equilibration process

Initially, 200,000 time steps of the equilibrium behavior of aluminum polycrystal were examined. Using a Nose-Hoover thermostat with a 0.1 temperature damping ratio, the initial temperature was adjusted to 300 K. This stage calculated the temperature and potential energy changes as a function of simulation duration until equilibrium phase detection. The temperature of polycrystal converges to 300 K after 200,000 time steps, as Fig. 2 illustrates. This atomic development anticipated the atomic unity among different crystal areas within the sample and within the sample structurally. The potential energy change throughout the equilibration process is seen in Fig. 3. In the equilibrium phase, this energy reached a numerical convergence of −3.371 eV at the last time step. The mean attraction force among different particles within the computational box was anticipated physically by the potential energy's convergence to the negative value in this computational phase. The potential energy convergence in the equilibration process demonstrated that the simulation reached a stable state where the potential energy of the system no longer exhibited significant fluctuations. This

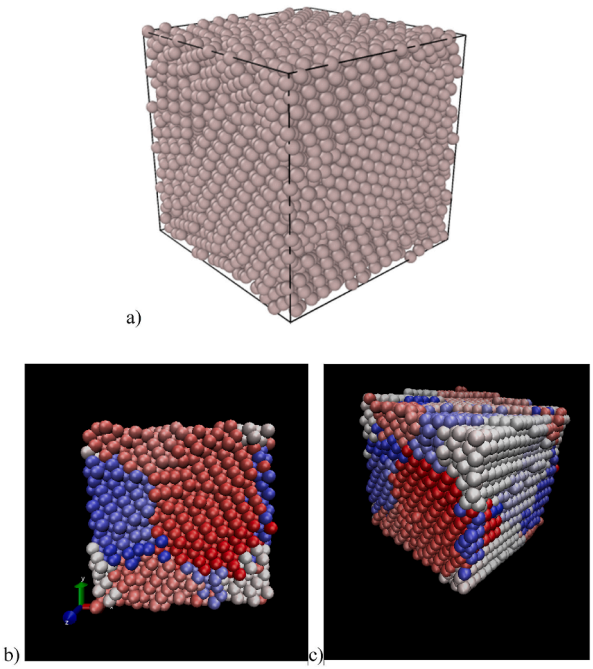


Fig. 1. A schematic of a)the simulated structure (In this Fig, the Al atoms represented with gray color) and b)different grains are distinguished by different colors via the VMD software from b) front and b)perspective view. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

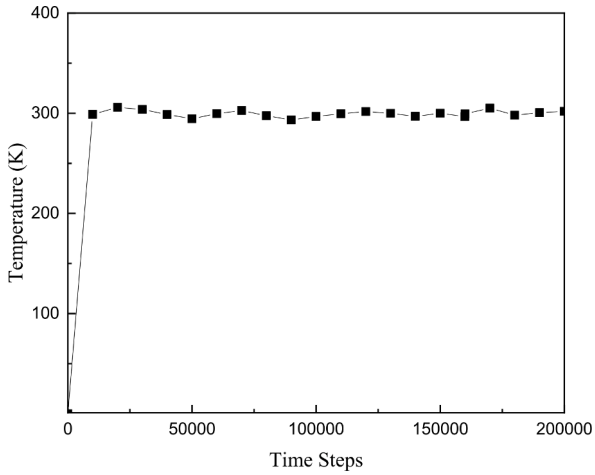


Fig. 2. The change in the temperature of simulated aluminum polycrystal.

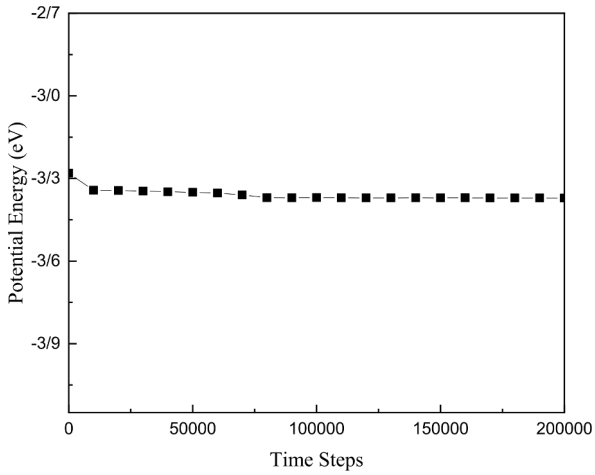


Fig. 3. The change in the potential energy of simulated aluminum polycrystal.

indicated that the system achieved a thermodynamically consistent configuration, reflecting the adequacy of the simulation time, appropriate settings, and the accuracy of the force field used. A well-converged potential energy signifies that the system equilibrated effectively, allowing for reliable and meaningful analysis of its properties and behavior. Also, this atomic performance of aluminum polycrystal predicts the appropriate MD settings in current research, as reported before [30,31].

2.3. Radial distribution function (RDF)

To validate the MD approach in the mechanical behavior description of Al polycrystal, the RDF of this sample was calculated after equilibrium phase detection. RDF is a metric used to characterize the spatial arrangement of atoms in atomic polycrystals. The information it gives pertains to the likelihood of locating an atom at a certain distance from a reference atom inside the crystal structure. RDF quantifies the spatial configuration of atoms. It offers information on the specific arrangement of atoms in the immediate area, such as the number of neighboring atoms, the distances between atoms, and the level of organization within the polycrystalline material. MD result for the RDF parameter of equilibrated Al polycrystal (at 300 K) is depicted in Fig. 4. The various peaks in this output predicted the sample's solid phase and structural unity. Furthermore, this sample's pattern is consistent with previous structural reports [32]. This consistency validates the implemented computational approach in current work.

3. Results and discussion

The mechanical test settings were implemented to design Al polycrystal by the equilibrium phase inside the sample. Their structural expansion with a 1 s-1 strain value was occurred in this mechanical test. This expansion is depicted in Fig. 5. This atomic representation was created using OVITO software [33]. Structurally, the graphical outputs of the mechanical test in this step predicted the atomic stability of the sample in the mechanical test procedure. So, our modeled Al polycrystal can be effectively used for various mechanical applications.

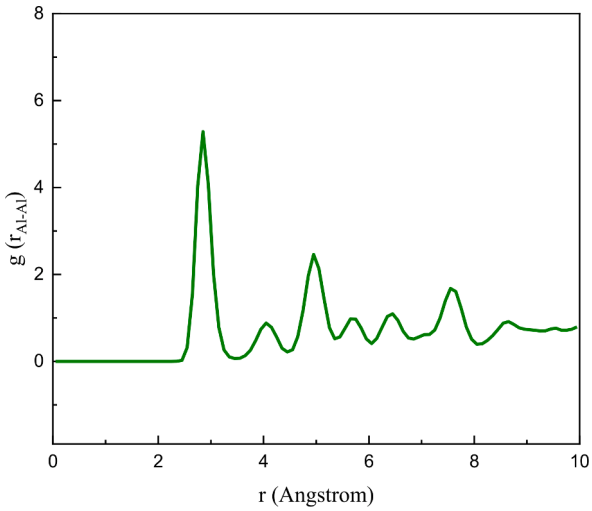


Fig. 4. The RDF of the atomic system after the equilibrium process.

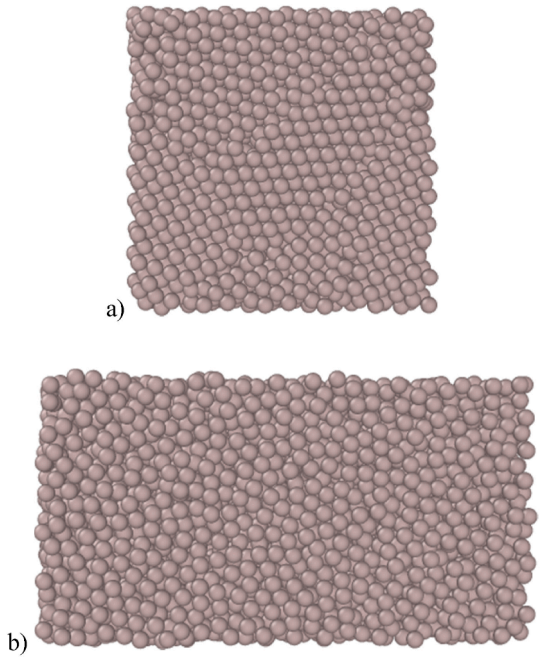
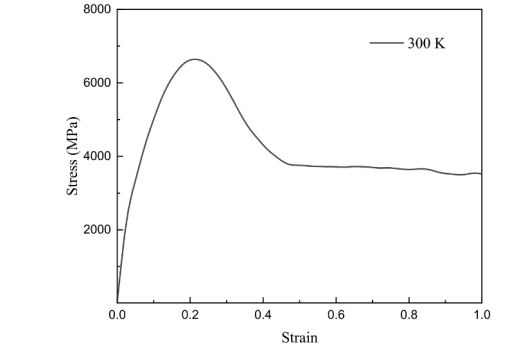


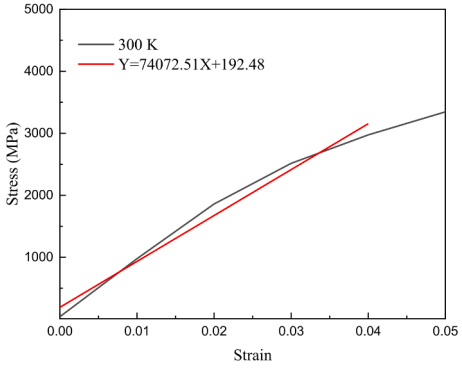
Fig. 5. The mechanical test of the simulated Al polycrystal at the a) first and b) final time steps.

Through the application of structural expansion parameters to an equilibrated Al polycrystal, their stress-strain curve may be determined. The connection between applied stress and resultant strain in a polycrystalline material is described by the polycrystal stress-strain curve. The material deforms when stress was applied, and the stress-strain curve illustrated how the material reacted to this deformation. Typically, the curve was composed of many separate zones, such as failure, plastic deformation, and elastic deformation. So, valuable mechanical results can be estimated using this curve of polycrystals. This curve of equilibrated Al polycrystal at 300 K (as initial temperature) is shown in Fig. 6a. The mechanical output pattern illustrates the average force of attraction among different particles in this sample. Numerically, the sample's US and YM converged to 6.640 and 74.072 GPa, respectively. The YM of this sample is depicted in Fig. 6b.

The effects of initial temperature on the mechanical performance of Al polycrystals are investigated in the next phase. In their equilibrium phase, the initial temperature was changed for this purpose from 350 to 450 K. Fig. 7 shows the stress-strain and YM results for these samples. The mechanical performance of an Al polycrystal tuned at various temperatures was anticipated from these results. Physically, increasing initial temperature caused the atomic mobility of samples to increase. This performance occurred by the amplitude of atomic displacement increasing in higher temperatures. Structurally, this described process can both improve mechanical resistance and weaken it. The atomic locations in the inter-crystalline regions of polycrystals were enhanced by raising the initial



a)



b)

Fig. 6. The a)stress-strain curve and b) YM of the Al polycrystal at 300 K.

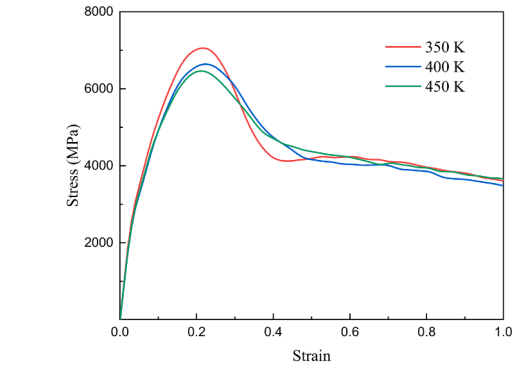
temperature. Hence, over the whole sample, the attraction force grew. The interatomic distance increased with further temperature rises. The mean distance between atoms and the potential energy, often known as the interatomic force, are reciprocal. As a result, both mechanical behavior and the interatomic attraction force diminish as a result of the secondary temperature rise.

The numerical changes of US and YM of Al polycrystals at different initial temperatures were reported in the final step of our MD simulations. The US, which stands for the utmost stress a polycrystalline substance can endure prior to failure or fracture, is a characteristic of polycrystals. Young's modulus (YM) in atomic structures, commonly referred to as the elastic modulus, quantifies the degree of stiffness or rigidity exhibited by a material on the atomic scale. It specifies the resistance of the material to deformation under the effect of an external force. YM measures the correlation between strain and stress within an atomic structure. As shown in Figs. 8 and 9 and Table 1, with increasing temperature from 300 to 350 K, the US and YM of the designed Al polycrystal increased from 6.640 to 74.072 GPa to 7.055 and 79.226 GPa respectively. The observed increase in US and YM of the designed aluminum polycrystal as the temperature increased from 300 to 350 K can be attributed to the enhanced thermal activation of dislocation motion and the increased mobility of atoms at higher temperatures. The increased values of US and YM were partly explained by the better material strength and stiffness that follow from a more effective dislocation contact and movement. The increased thermal activation of dislocation motion and the increased atomic mobility at higher temperatures are responsible for the reduction in US and YM of the aluminum polycrystal as the temperature rises to 450 K. This increased thermal energy promoted more pronounced dislocation movement and interaction, leading to a reduction in material strength and stiffness, resulting in the observed decrease in US and YM values. All of our numerical (mechanical) outputs are listed in Table 1.

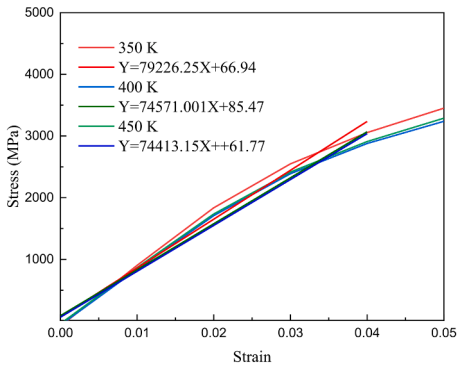
4. Conclusion

Aluminum (Al) polycrystals are advantageous materials for a wide range of applications in the aerospace, automotive, construction, and manufacturing sectors due to their exceptional mechanical properties. Young's modulus (YM) and ultimate strength (US) are investigated by employing a molecular dynamics (MD) methodology. The present investigation employed the to characterize the effects of initial temperature on their mechanical performance. Main MD outputs from these phases can be listed as below.

- The results show that potential energy and temperature convergence to −3.371 eV and 300 K fter 200,000-time steps. This convergence indicated that the system achieved a thermodynamically consistent configuration, reflecting the adequacy of the simulation time, appropriate settings, and the accuracy of the force field use



a)



b)

Fig. 7. A) The stress-strain curve and b) YM of the Al polycrystal with increasing temperature.

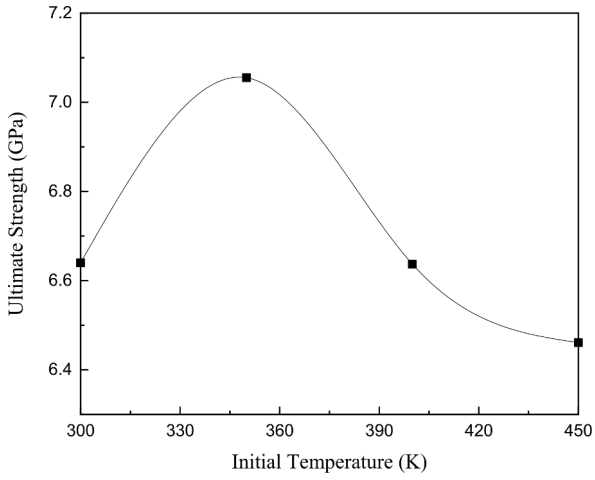


Fig. 8. The US variation of the Al polycrystal with increasing initial temperatures.

- Numerically, by increasing temperature from 300 to 350 K, the US and YM of the designed Al polycrystal increase from 6.640 to 74.072 GPa to 7.055 and 79.226 GPa, respectively. This led to a more efficient dislocation interaction and movement, resulting in improved material strength and stiffness, thus contributing to the higher values of US and YM
- By furthere increasing temperature to 450 K, US and YM decrease to 6.461 and 74.413 GPa, respectively. This decrease can be attributed to the intensified thermal activation of dislocation motion and the greater mobility of atoms at higher temperatures.

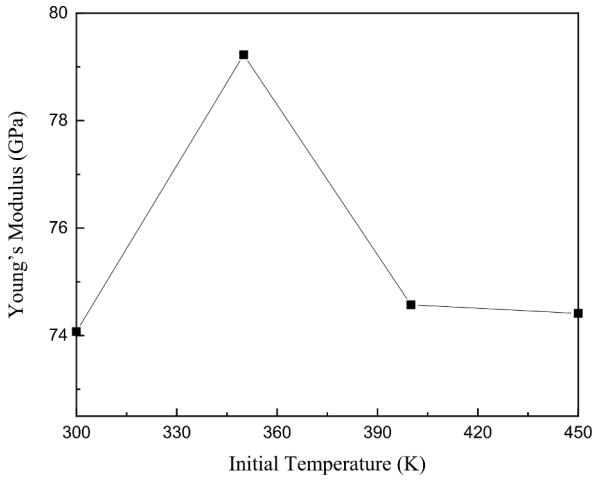


Fig. 9. YM variation of the Al polycrystal with increasing initial temperatures.

Table 1
YM and US variation of the simulated Al polycrystal at various temperatures.

Temperature (K)	US (GPa)	YM (GPa)
300	6.640	74.072
350	7.055	79.226
400	6.637	74.571
450	6.461	74.413

The proposed solution holds significant importance in optimizing the performance of aluminum polycrystals for aerospace, automotive, construction, and manufacturing applications. By examining the effect of temperature on the material's ultimate strength and Young's modulus, the research offerred valuable insights for enhancing material performance under various environmental conditions. These findings not only inform engineering design and reliability, but also have the potential to drive cost and resource efficiency in manufacturing processes. Moreover, the study contributed to broader scientific understanding of material behavior at the atomic level, making it a valuable addition to the field of materials science and engineering.

CRediT authorship contribution statement

Peng Lin: Supervision, Writing – review & editing, Conceptualization, Data curation, Formal analysis. **Ali Basem:** Supervision, Writing – review & editing, Conceptualization, Data curation, Formal analysis. **As'ad Alizadeh:** Writing – review & editing, Conceptualization, Data curation, Formal analysis. **Eissa N. Nasser:** Supervision, Writing – review & editing, Conceptualization, Data curation, Formal analysis. **Mohammed Al-Bahrani:** Investigation, Writing – original draft. **Choon Kit Chan:** Investigation, Writing – original draft. **Nafiseh Emami:** Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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