YTUP

Journal of Thermal Engineering
https://jten.yildiz.edu.tr/
https://doi.org/10.47481/jten.0069

RESEARCH ARTICLE

# Thermodynamic stability in Cu–Ta functionally graded materials using molecular dynamic simulation

Dhowmya Bhatt[1,*], Nagajyothi Koripella[2]

[1]Department of Computer Science Engineering, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Delhi NCR Campus, Ghaziabad, UP, 201204, India
[2]Pro Vice Chancellor, Bharatiya Engineering Science and Technology Innovation University, Andhra Pradesh, 515231, India

## Abstract

Molecular dynamics simulations were performed on copper-tantalum FGMs to investigate the mechanical and thermophysical under uniaxial tensile deformation. Molecular dynamics simulations were carried out to examine the influence of tantalum content, temperature, and strain rate on mechanical response, plastic deformation mechanisms, atomic mobility, and energy dissipation. The study focuses on analyzing the properties of one layer of pure copper and another layer of copper with tantalum content varying from 0% to 10%. The applied strain rate ranged from $10^8$ $s^{-1}$ to $10^{11}$ $s^{-1}$, and the temperature varied from 200 K to 1000 K in intervals of 200 K. This study offers valuable insights into the high-temperature plastic deformation and thermodynamic behavior of Cu-Ta FGMs. At elevated temperatures, the plastic deformation mechanism accelerates atomic diffusion and enhances thermal energy transport, thereby minimizing dislocation density and flow stress. This study offers fundamental insights into the high-temperature deformation and heat-transfer characteristics of Cu–Ta FGMs, supporting their potential applications in biomedical and aerospace thermal systems. Increasing the Ta content promotes plastic activity within grains and at grain boundaries at low temperatures, while at higher temperatures the plastic and thermal deformation mechanisms stay like those before Ta addition. The novelty of this study lies in the combined analysis of mechanical response, thermodynamic parameters, and atomic mobility in Cu-Ta FGMs under extreme thermo-mechanical loading, offering new insights into high-temperature plasticity and energy transport mechanisms. This integrated understanding has not been reported previously and directly supports the development of Cu-Ta FGMs for advanced biomedical and aerospace thermal applications. These findings contribute to an improved understanding of the coupled thermo-mechanical and thermodynamic behavior of Cu-Ta FGMs at the nanoscale and inform the design of novel materials with tailored mechanical and heat-transfer properties.

**Keywords:** Temperature, thermal stress, energy dissipation, copper-tantalum, molecular dynamic simulation, functionally graded materials, nanomaterials

**Cite this article as:** Bhatt, D., & Koripella, N. (2026). Thermodynamic stability in Cu–Ta functionally graded materials using molecular dynamic simulation. Journal of Thermal Engineering, 12(5), 1837–1847. https://doi.org/10.47481/jten.0069

## 1. Introduction

The importance of functionally graded materials (FGMs) has increased due to the delamination issues commonly seen in conventional composite materials. FGMs are advanced engineering materials composed of more than one constituent phase, in which the material composition varies gradually across the structure. [1]. Functionally graded materials (FGMs) are potential substitutes for conventional materials applications that involve severe operating conditions, such as turbine blades, coatings, heat-exchanger tubes, and biomedical implants. Coatings are layers applied to a substrate. Under harsh working conditions, interlaminar stresses between the substrate and the coating cause the coating to wear or detach from the substrate. This wear or the peeling of coatings results mainly from the abrupt mismatch of material properties between the coating and the substrate. FGMs help to overcome these issues because they have a smooth spatial gradation of material constituents. As a result, FGMs are promising candidates for emerging applications such as artificial bones,

*Corresponding Author
E-mail Adress: bhattdresearch@gmail.com

**Submitted:** 11 November 2025; **Accepted:** 19 June 2026

This paper was recommended for publication in revised form by Editor-in-Chief Ahmet Selim Dalkılıç

artificial skin, thermoelectric generators, and sports equipment. [1,2]. FGM initially developed with the purpose of keeping temperature difference between internal and outer layer of spacecraft [3,4]. Functionally graded materials are the prime materials for high temperatures applications like combustion chambers for reusable rockets [5,6].

Laminated metal composites with alternating layers prove unique mechanical advantages over conventional pure metals or alloys [7]. Copper-tantalum nanomaterials are well suited for medical applications due to specific material properties such as biocompatibility, antibacterial activity, and promotion of bone ingrowth [8-12]. Although not all such properties are present, several challenges related to mechanical properties need to be addressed. As per the earlier studies, some important consideration for designing are mechanical properties that need to be taken carefully such as Young's modulus, yield strength, and ultimate tensile strength (UTS) [13,14] and during accident loosening of implants.

Earlier researchers mentioned that nature of Cu-Ta, grain size, density of grain boundaries (GBs), stacking faults (SFs), etc are the crucial factors which need to be addressed to investigate the real problem of nanomaterials for the purpose of dental implants [14-16]. The dynamic behavior of Flax/E-glass hybrid composite plates was investigated using experimental modal analysis and FSDT-based finite element modeling to examine the effects of boundary conditions, ply angle, and aspect ratio; experimental and MATLAB results showed good agreement. Ceramic-coated exhaust manifolds ($TiO_2$, $ZrO_2$, $Al_2O_3$) deposited via plasma arc showed enhanced thermal performance and reduced residual stresses, with $Al_2O_3$ providing the best overall performance [17-19].

Apart from the aforementioned factors, strain rate is an important parameter to consider in the development of dental implants. Earlier studies have revealed that mechanical behavior is significantly influenced by strain rate at different stages, such as implant design, fabrication, post-surgical conditions, and in-service performance within the human body [20-22]. Al 7075–based metal matrix composites reinforced with 2-8 wt.% $Al_2O_3$ were fabricated using stir casting followed by heat treatment to enhance impact strength and hardness [23-25]. Numerous studies have concluded that strain rate is a crucial parameter influencing the mechanical behavior of materials used in polycrystalline-based implants [26,27]. Zhou et al. [28] investigated the Cu/Ta-based interfacial region and examined the effect of strain rate, concluding that an increase in strain rate enhances interfacial activity, resulting in dislocation transfer between the phases.

Molecular dynamics simulation is employed to investigate atomic-scale phenomena and is a powerful tool for exploring the strain-rate-dependent microstructural evolution in nanostructured FGM [29-31]. Using molecular simulation Pan et al [32]. investigated the fine grain sample of Ta and reported that flow stress showed the strongest correlation with strain rate, showing a shift in plastic deformation mechanisms at different strain levels. Hahn et al [33] investigated Ta with molecular dynamic simulation and reported that at low strain rates of $10^7$ - $10^{10}$ $s^{-1}$, plastic deformation is mainly due to deformation slip and at higher strain rates $10^{13}$ $s^{-1}$, responsible mechanism for plastic deformation is grain boundary decohesion leads to failure. Recent studies have proved that nano-enhanced phase-change materials significantly improve thermal transport and energy-storage performance by enhancing thermal conductivity and phase-change behavior. Furthermore, tri-hybrid nanofluids and graphene oxide–based systems show superior heat transfer and increased entropy generation, highlighting complex thermodynamic irreversibility and energy dissipation mechanisms. These findings collectively emphasize the critical role of nanoparticle interactions and thermal transport coupling [34-37]. Cu-Ta FGMs subjected to different strain rates and showing plastic deformation mechanisms at various temperatures have rarely been investigated at the atomic scale. The mechanisms of plastic deformation in nanomaterial, making them difficult to investigate experimentally.

Several earlier studies have investigated the mechanical behavior of Cu-Ta alloys and multilayered systems under different strain rates and temperature conditions. Earlier molecular dynamics investigations have primarily focused on tensile behavior, dislocation evolution, grain-boundary activity, strain-rate sensitivity, and deformation mechanisms in conventional Cu-Ta nanoalloys or multilayer structures. However, limited attention has been given to Cu-Ta functionally graded materials (FGMs), particularly about the coupled thermo-mechanical and thermodynamic behavior under simultaneous temperature and strain-rate variations. In addition, the combined influence of plastic deformation, atomic mobility, defect evolution, and energy dissipation mechanisms in graded Cu-Ta systems at the nanoscale has not been comprehensively explored. The present study differs from earlier investigations in that it examines a functionally graded Cu-Ta configuration with gradual compositional variation using molecular dynamics simulations across a wide range of temperatures and strain rates. Earlier studies that primarily focused on isolated mechanical responses. Furthermore, advanced structural analysis techniques, including Polyhedral Template Matching (PTM), Dislocation Extraction Algorithm (DXA), Centro-Symmetry Parameter (CSP), and grain segmentation analysis, are employed to gain deeper insights into deformation and defect mechanisms. This comprehensive approach provides a new understanding of the coupled thermo-mechanical response of Cu-Ta FGMs and supports their potential application in advanced biomedical and aerospace thermal systems. This investigation aims to understand the coupled thermo-mechanical and thermodynamic behavior of Cu-Ta functionally graded materials at the nanoscale. Molecular dynamics simulations were carried out to examine the influence of tantalum content, temperature, and strain rate on mechanical response, plastic deformation mechanisms, atomic mobility, and energy dissipation. This study offers fundamental insights into the high-temperature deformation and heat-transfer characteristics of Cu-Ta FGMs, thereby supporting their potential application in aerospace thermal systems.

To investigate the mechanical response of the Cu-Ta functionally graded material (FGM), simulations were carried out under five different temperature conditions (200, 400, 600, 800, 1000) at a fixed strain rate of $1\times10^{9}$ $sec^{-1}$. In addition, at a constant temperature of 400 K, the strain rate was varied from $1 \times 10^{8}$ $sec^{-1}$ to $1 \times 10^{11}$ $sec^{-1}$.

## 2. Simulations methodology

The present study employed MD simulations to investigate Cu-Ta FGM at different strain rates and temperatures. The applied strain rates are significantly higher than experimental loading conditions due to the intrinsic time-scale limitations of MD simulations; however, such strain rates are commonly adopted to investigate atomistic deformation mechanisms within computationally possible timescales. Furthermore, the Cu-Ta FGM model consists of an idealized nanoscale structure with controlled compositional grading and limited first defects, while real engineering materials may show microstructural heterogeneity, impurities, residual stresses, and manufacturing-induced imperfections. Therefore, the present results should primarily be interpreted as offering qualitative insight into the fundamental thermo-mechanical and deformation mechanisms governing Cu-Ta FGMs at the nanoscale. The dimensions of the simulation model were chosen to balance computational efficiency and the correct representation of nanoscale deformation mechanisms. The model, which consists of 128,000 atoms - 50% of the specimen composed of pure Cu and the remaining 50% consisting of Cu-10%Ta with a linear compositional gradient sufficiently large to capture dislocation nucleation, grain boundary evolution, interface interactions, and thermally activated atomic motion during tensile deformation. The relatively small thickness of 2 nm was chosen to reduce computational cost while preserving the essential atomistic mechanisms governing the thermo-mechanical response of the Cu-Ta FGM system. Similar nanoscale dimensions and thicknesses have been widely used in earlier molecular dynamics investigations of metallic multilayers and nanostructured materials. Periodic boundary conditions were applied in all three directions to minimize artificial free-surface effects and to approximate bulk material behavior during deformation. In the present Cu-Ta functionally graded system, periodicity ensures continuity of atomic interactions and avoids nonphysical edge-stress concentration effects that could influence deformation behavior. The graded Cu-Ta interface was constructed by a compositional transition from pure Cu to Cu-10%Ta regions to minimize abrupt lattice mismatch and interfacial instability. This compositional gradient reduces localized stress concentrations and promotes stable interfacial bonding between the FCC Cu and BCC Ta phases. Prior to tensile loading, the structure was subjected to energy minimization using the conjugate-gradient method to cut residual stresses and unstable atomic overlaps near the interface and grain-boundary regions. After minimization, the system was equilibrated to obtain a thermodynamically stable atomic configuration before applying uniaxial tensile strain. This relaxation process ensures that the observed deformation behavior originates from the intrinsic thermo-mechanical response of the Cu-Ta FGM rather than from other sources, artificial first stress effects. The model consists of 128,000 atoms, 50% of the specimen is composed of pure Cu, and the remaining 50% is composed of Cu-10%Ta with a linear compositional gradient. The structure includes one Cu crystal with a face-centered cubic (FCC) lattice and one Ta crystal with a body-centered cubic (BCC) lattice, with lattice parameters of 3.615 Å and 3.306 Å, respectively. Table 1 is the simulation parameters used in the present study.

**Table 1.** Simulation Parameters for Cu-Ta FGM

| Parameters | Specifications |
|---|---|
| Number of atoms | 128,000 |
| Timestep | 1 fs |
| Boundary conditions | Periodic in all three Direction |
| Potential | Embedded Atom Method |
| Strain rate variations ($sec^{-1}$) | $1\times10^{8}$, $1\times10^{9}$ ,$1\times10^{10}$ ,$1\times10^{11}$ |
| Temperature variations (K) | 200, 400, 600, 800, 1000 |

### 2.1. Simulation model, and interatomic potential

The present MD simulations are influenced by several modeling parameters, including the choice of interatomic potential, timestep size, boundary conditions, strain rate, and simulation domain dimensions. The EAM potential employed in this work has been previously confirmed for Cu-Ta systems and metallic nanostructures, providing reliable predictions of deformation and thermodynamic behavior. A time step of 1 fs was used to keep numerical stability during tensile loading. Although the absolute quantitative values may vary with simulation scale and loading conditions, the observed trends in mechanical response, defect evolution, and temperature-dependent plasticity remain consistent across the investigated conditions, supporting the qualitative robustness of the present model. However, uncertainties associated with nanoscale dimensions and high MD strain rates should be considered when comparing with bulk-scale experimental behavior. In the current study, the simulation model dimensions in the x and y directions were 16 × 16 nm, with a thickness of 2 nm in the z direction. A uniaxial tensile simulation test is performed in the x direction. An energy minimization method was used to remove prestress in the materials. To avoid overlap between grain boundaries, the conjugate gradient method for energy minimization is employed at grain boundaries. Interatomic potential plays the most significant role.

In present study, potential developed by Zhou et al 2004 [38] was used for the simulation process. The interatomic potential, the embedded atom method (EAM), and the conjugate gradient method for energy minimization were important parameters in the present simulation.

### 2.2. Simulation and visualization software packages

MD simulation was completed with the help of large-scale atomic/molecular massively parallel simulator (LAMMPS) [39]. The OVITO software was used to analyses the microstructure and visualize the Cu-Ta FGM sample prepared for the tensile test. OVITO (Open Visualization Tool) is a widely used, open-source software package for the post-processing, visualization, and analysis of atomistic simulation data generated by molecular dynamics simulations. In the present study, OVITO was employed to visualize the atomic configurations and analyze deformation mechanisms in Cu–Ta functionally graded materials during uniaxial tensile loading. The software enables detailed structural analysis through tools such as common neighbor analysis (CNA), centrosymmetric parameter (CSP), and dislocation extraction algorithms (DXA), which help find crystal structures, defects, dislocations, grain boundaries, and stacking faults. OVITO also eases the evaluation of atomic displacement, local strain distribution, and temperature-dependent atomic mobility, offering clear insight into plastic deformation and thermodynamic behavior at the nanoscale. Its robust visualization and quantitative analysis capabilities make OVITO an effective tool for interpreting the mechanical and thermo-physical responses seen in MD simulations. [40]. In all simulations, the crystal structure was examined using common neighbor analysis (CNA) and dislocation length variations and interactions were studied using DXA. The samples were generated using the three-dimensional Voronoi tessellation method [41]. Monitoring the sample after phase transition was seen by the Polyhedral Template Matching (PTM) [42]. In present study Centro-Symmetry Parameter (CSP) analysis was used to find the defects and dislocations in the sample after tensile test [43].

Figure 1 depicts the Cu-Ta FGM structure before and after minimization. The copper–tantalum sample was prepared with 50% pure copper, and the remaining 50% as a functionally graded material composed of 90% copper and 10% tantalum, with the percentage of tantalum varying from the center to the extreme right corner. Figure 1 (a) is the Cu-Ta FGM before minimization, but Figure 1 (b) is the Cu-Ta FGM after minimization and relieving pre-stress. Figure 1(c) is the Cu-T FGM, after a certain applied strain; stress generation transforms the single-crystalline structure into a polycrystalline one. In Figure 1(c), the right side of the Cu-Ta FGM has 11 grains, which is attributable to significant deformation in that region of the sample. The unstrained structure in Figure 2(a) and the strained structure in Figure 2(b) are the structures before and after deformation up to 0.11% strain and help to clarify changes in the materials' atomic structure.

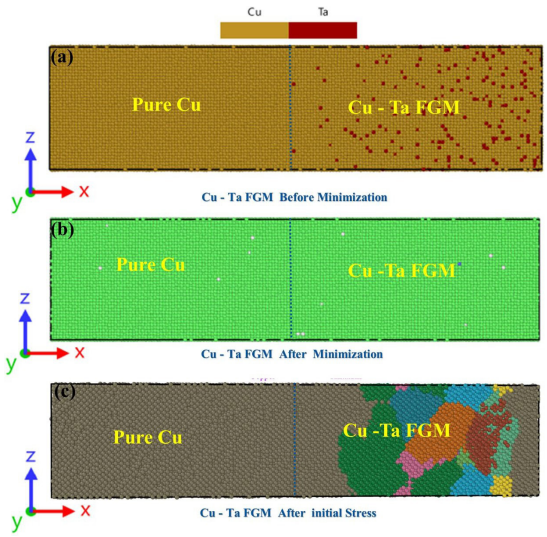



**Figure 1.** Cu-Ta FGM structure **(a)** before minimization **(b)** after minimization **(c)** after application of stress

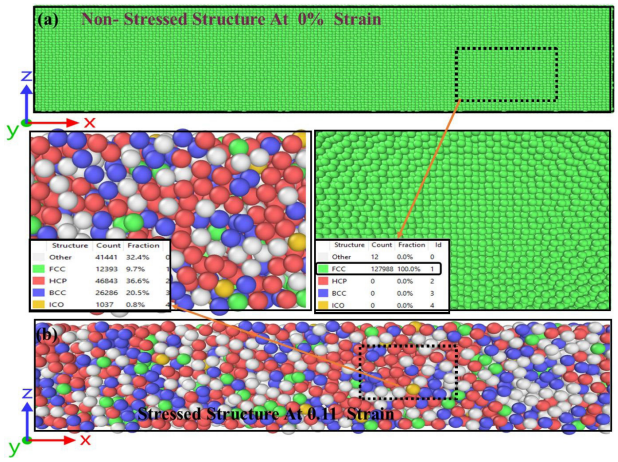



**Figure 2.** Cu-Ta FGM structure different strain level **(a)** unstrained structure at 0% **(b)** strained structure at 0.11%

In Figure 2(b), the Ackland-Jones analysis is used to find local atomic structures based on their local bonding mechanisms in the Cu-Ta FGM. The different structure of the Cu-Ta FGM can be seen in Figure 2(b). Nanoscale systems typically show behaviors such as, higher clear strength, enhanced strain-rate sensitivity, limited dislocation activity, grain boundary-dominated deformation mechanisms, which may differ quantitatively from bulk material behavior due to the reduced dimensions and extremely high strain rates inherent to MD simulations. Despite these scale limitations, MD simulations stay highly valuable for revealing the underlying atomistic mechanisms governing deformation and energy dissipation, which are often difficult to see experimentally. The trends seen in the present work, such as the reduction in strength with increasing temperature and the increase in resistance at higher strain rates, remain physically meaningful and qualitatively consistent with experimentally seen metallic behavior.

### 2.3. Validation of present model with benchmark model

A simulation was performed to confirm the present model against available results in the literature. Similar parameters were used for the simulation as those adopted by Gupta et al. [44], such as periodic boundary conditions, a temperature of 300 K, a strain rate of $1 \times 10^{-9}$, a time step of 1 femtosecond, and the EAM potential.

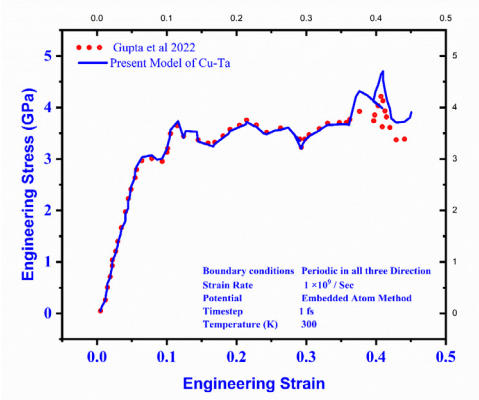



**Figure 3.** Validation of the present model with existing MD model Gupta et al [44]

Figure 3 shows that the present model is in good agreement with the Gupta et al. model, which confirms the reliability of the simulation approach. However, an error of 1.5% was seen in the fracture and neck zones, which is within an acceptable range. This error arises from variations in the number of atoms in the current model. The percentage variation of the calculated mechanical properties was small and did not significantly affect the overall thermo-mechanical trends or deformation mechanisms saw in the study. The dominant deformation features, including dislocation nucleation, grain boundary activity, and defect evolution, remain consistent across repeated simulations. Potential sources of uncertainty such as thermal noise, local atomic rearrangement, and sensitivity to first atomic configurations are inherent to molecular dynamics simulations but can be minimized by energy minimization and equilibration prior to loading.

These results confirm the robustness and reliability of the present simulation method for investigating the thermo-mechanical behavior of Cu-Ta functionally graded materials. The reliability of the present MD framework is supported not only through direct benchmark comparison with published results, but also through the consistency of the obtained thermo-mechanical trends and deformation mechanisms with previously reported atomistic studies on Cu-Ta systems. The adopted EAM potential and simulation method have been widely used to investigate plastic deformation, strain-rate sensitivity, and thermodynamic behavior in metallic nanostructures, thereby supporting the robustness of the present simulations under the investigated loading conditions. The mechanical properties obtained and deformation trends are in reasonable agreement with previously reported MD studies of Cu-Ta and nanocrystalline Ta systems. The observed increase in flow stress with strain rate and reduction in strength with increasing temperature are consistent with the findings reported by Gupta et al. [14-16,27], Pan et al. [32], and Hahn et al. [33]. Furthermore, the deformation mechanisms involving dislocation evolution, grain boundary activity, and thermally activated atomic mobility qualitatively agree with earlier atomistic investigations. The mechanical properties predicted in the present study are in good agreement with earlier molecular dynamics investigations of Cu–Ta systems and nanocrystalline tantalum. Gupta et al. [14-16] reported yield strength values in the range of approximately 3-6 GPa for Cu-Ta nanoalloys under varying strain-rate and temperature conditions, which is comparable to the present predicted yield strength values ranging from 3.6 GPa to 8.72 GPa depending on strain rate. Similarly, Pan et al. [32] saw significant strain-rate strengthening in nanocrystalline tantalum, where the flow stress increased considerably with increasing loading rate due to restricted dislocation mobility, which is consistent with the present findings. The predicted Young's modulus values in the present work (36-54 GPa) are consistent with earlier atomistic studies of Cu-based nanostructured systems, which show that elastic stiffness increases under higher strain-rate loading conditions. Hahn et al. [33] reported that deformation behavior in tantalum transitions from dislocation-mediated plasticity to grain-boundary-dominated failure mechanisms at extremely high strain rates, which correlates well with the increased defect accumulation and rapid stress evolution seen in the present Cu-Ta FGM simulations.

## 3. Result and discussion

In the present study, MD simulations were used to investigate the behavior of Cu-Ta FGM. The sample has been constructed in such a manner as to see the functionally graded properties of Cu-Ta. Uniaxial tensile test is performed in the x-direction. Direction to see the change in the plastic deformation at a range of temperature scale 200 K, 400 K, 600 K, 800 K, and 1000 K.

### 3.1. Mechanical properties variation with strain rates and fixed temperature 400K

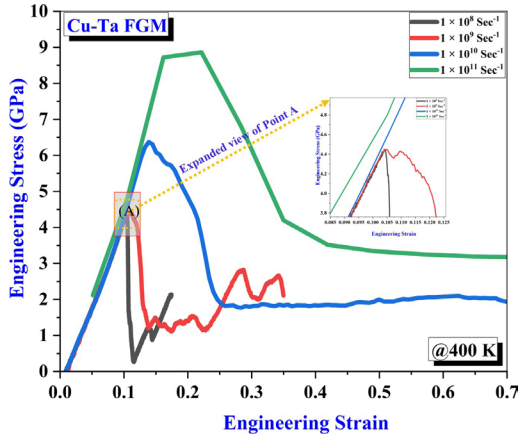



**Figure 4.** Engineering stress and engineering strain with strain rate variation and at fixed temperature of 400 K

Figure 4 depicts the relation between engineering stress and engineering strain at 4 different strains rates $1 \times 10^8$ $sec^{-1}$, $1 \times 10^9$ $sec^{-1}$, $1 \times 10^{10}$ $sec^{-1}$, and $1 \times 10^{11}$ $sec^{-1}$. In figure 4, at maximum strain rate $1 \times 10^{11}$ $sec^{-1}$ the engineering stress reaches to 8.86 GPa and minimum engineering stress at $1 \times 10^8$ $sec^{-1}$ is 4.19 GPa. A temperature of 400 K was selected for detailed microstructural and deformation analyses because it is an intermediate thermo-mechanical condition in which both mechanical resistance and thermally activated deformation mechanisms coexist. This temperature range is also relevant to several engineering applications involving localized thermal exposure, thermal management systems, and elevated-temperature service environments. Moreover, the broader temperature range investigated in the present study (200-1000 K) was intended to capture the transition in deformation behavior from low-to high-temperature regimes. Temperature strengthening to high-temperature plasticity. In MD simulations employing periodic boundary conditions and homogeneous deformation, the stress-strain representation is the standard and physically meaningful metric. At point A, all four graphs overlap; to visualize this, an expanded view of this section is presented in Figure 4.

The stress-strain response of the Cu-Ta FGM at 400 K shows a strong dependence on strain rate, as shown in Figure 4. The peak stress increases significantly with strain rate, rising from approximately 4.4 GPa at $10^8$ $s^{-1}$ to about 8.8 GPa at $10^{11}$ $s^{-1}$, showing pronounced strain-rate hardening. At lower strain rates ($10^8$-$10^9$ $s^{-1}$), the material shows a sharp drop in stress at once after the peak, suggesting the early onset of necking and localized deformation characteristic of relatively brittle behavior. At higher strain rates, the limited time available for dislocation relaxation and defect rearrangement increases the resistance to plastic deformation, resulting in higher flow stress and delayed stress softening on the MD timescale. Conversely, lower strain rates allow greater dislocation mobility and localized strain accumulation, promoting earlier stress drop and deformation localization. The strain-rate sensitivity coefficient (m) was estimated using the

$$m = d(\ln \sigma)/d(\ln \varepsilon) \quad \text{(i)}$$

Based on the peak stress values, the calculated m is approximately 0.10, which falls within the range of moderate strain-rate sensitivity (0.08-0.12). This suggests that the material shows noticeable resistance to deformation with increasing strain rate. The observed behavior can be attributed to the limited time available for dislocation motion and defect relaxation at higher strain rates, leading to increased resistance to plastic deformation. Conversely, at lower strain rates, dislocations have sufficient time to move and reorganize, resulting in early strain localization and reduced strength. At lower strain rates, atoms and dislocations have sufficient time to rearrange and accommodate the applied deformation through grain boundary sliding, defect annihilation, and localized stress relaxation. The material shows lower flow stress and an earlier onset of strain localization. Relatively longer deformation times promote thermally activated plasticity and ease progressive atomic redistribution within the graded Cu-Ta structure. In contrast, at higher strain rates, the available time for atomic diffusion and dislocation relaxation becomes significantly limited. This restriction suppresses defect recovery mechanisms and increases dislocation accumulation within the material, leading to enhanced strain hardening and higher peak stress. The rapid loading condition also promotes non-equilibrium deformation behavior, where stress concentration develops rapidly.

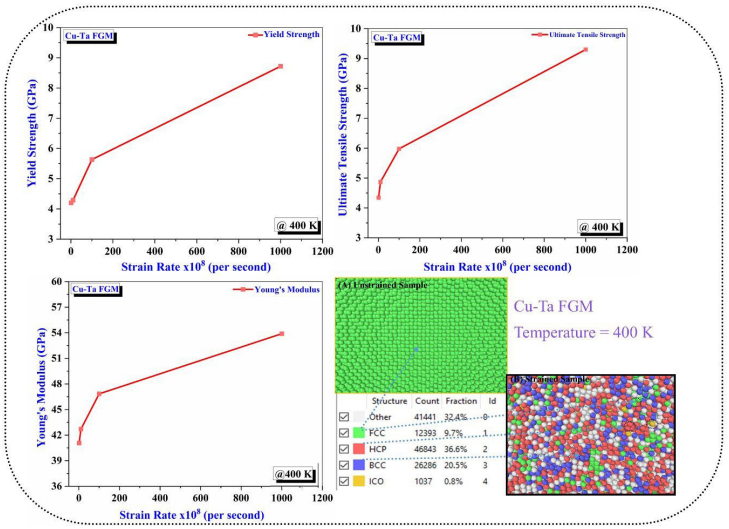



**Figure 5.** Mechanical properties with strain rate variation and at fixed temperature at 400 K

The material can accommodate plastic deformation through dislocation motion. Consequently, the Cu-Ta FGM shows increased resistance to deformation and delayed plastic relaxation at elevated strain rates. Furthermore, the addition of tantalum contributes to strain-rate strengthening through local lattice distortion and interface-controlled dislocation interactions. The mismatch between FCC Cu and BCC Ta structures generates interfacial stress fields that hinder dislocation propagation, particularly under rapid loading conditions. Therefore, the combined effects of limited atomic relaxation, defect accumulation, and Ta-induced interface strengthening govern the observed strain-rate sensitivity and thermo-mechanical response of the Cu-Ta functionally graded material.

At high strain rate, the materials do not have time to relax and difficult to achieve at experimental setup, so for the realistic approach a medium strain rate of, $1 \times 10^{10}$ $sec^{-1}$ is employed to investigate the plastic deformation mechanism, mechanical properties, microstructural examination, potential energy, kinetic energy, and defects analysis of the Cu-Ta FGM. Figure 5 is the Yield strength, Young's Modulus, and Ultimate tensile strength at all four $1 \times 10^8$ $sec^{-1}$, $1 \times 10^9$ $sec^{-1}$, $1 \times 10^{10}$ $sec^{-1}$, and $1 \times 10^{11}$ $sec^{-1}$ strain rates. As it can be depicted from figure, the middle range of strain $1 \times 10^{10}$ $sec^{-1,}$ is suitable to study at experimental setup. The properties at strain rate $1 \times 10^{10}$ $sec^{-1}$ are Yield strength, Ultimate tensile strength are 5.62 and 5.68 GPa, and Youngs modulus 46.84 GPa.

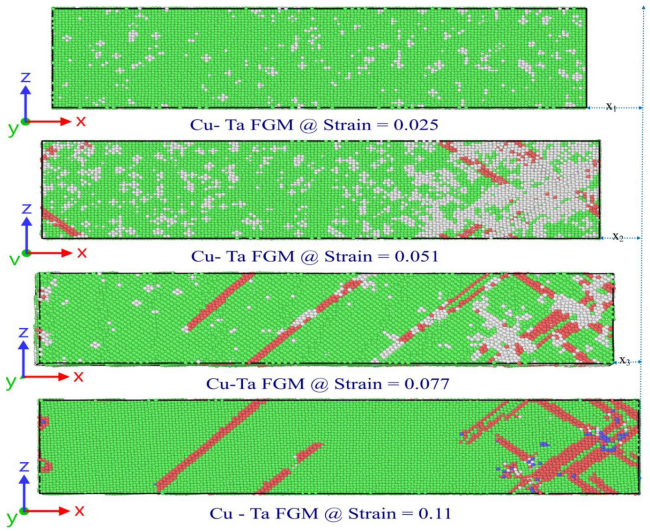



**Figure 6.** Polyhedral template matching of Cu-Ta FGM structure with strain at fixed temperature 400 K

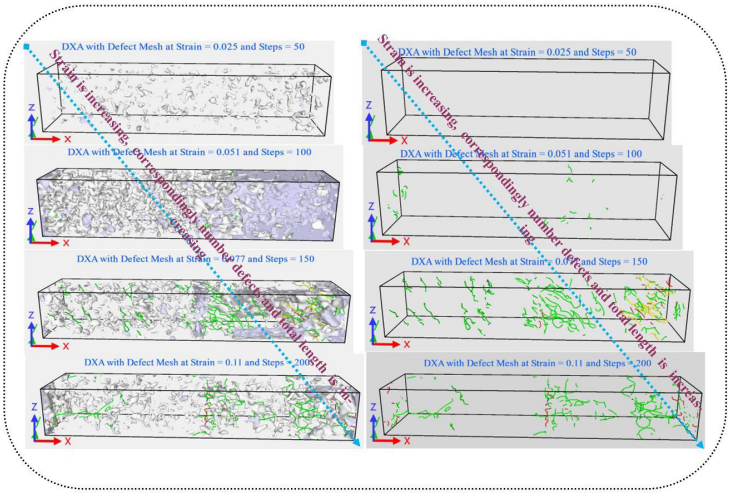
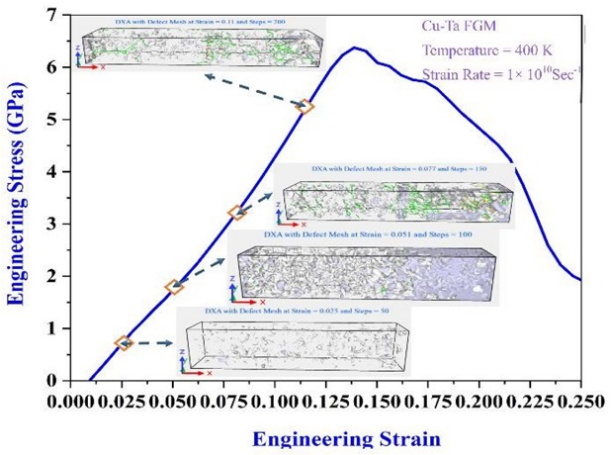



**Figure 7.** Dislocation extraction algorithm with and without mesh of Cu-Ta FGM structure

Figure 6 illustrates the Polyhedral Template Matching (PTM) of the Cu-Ta FGM structure under applied strain at a fixed temperature of 400 K. PTM helps accurately decide the local crystal orientation of atoms at grain boundaries, crystalline regions, interfaces, and free surfaces. At elevated temperatures, increased atomic vibrations enhance diffusion and accelerate dislocation activity, leading to increased energy dissipation. The graded distribution of tantalum changes lattice distortion and inhibits dislocation motion, thereby improving thermodynamic stability. In Figure 6, the Cu-Ta FGM sample is evaluated at four strain levels ranging from 0.025% to 0.11%. With increasing strain, the crystal structure undergoes changes, accompanied by increased defect generation and atomic misorientation. Figure 6 also illustrates that the length of the sample increases as the applied strain increases. Table 2 is the Yield strength, ultimate strength and Youngs modulus at 400 K.

**Table 2.** Is the yield strength, ultimate strength and Youngs modulus at 400 K

| Strain Rate ($Sec^{-1}$) | Youngs modulus (GPa) | Yield strength (GPa) | Ultimate strength (GPa) |
|---|---|---|---|
| $1 \times 10^{8}$ | 36.07 | 3.6 | 3.71 |
| $1 \times 10^{9}$ | 37.46 | 3.72 | 3.75 |
| $1 \times 10^{10}$ | 46.84 | 5.635 | 5.98 |
| $1 \times 10^{11}$ | 53.89 | 8.721 | 8.86 |



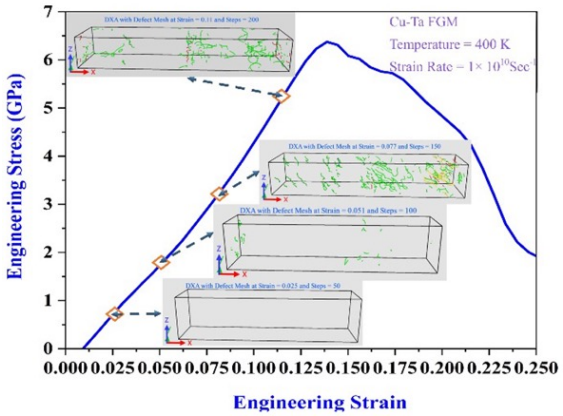




**Figure 8.** Dislocation extraction algorithm with stress – strain curve at fixed strain rate $1 \times 10^{10}$ $sec^{-1}$ and fixed temperature 400 K

In Figure 7, the Dislocation Extraction Algorithm (DXA) is used to find and characterize dislocations. The density of defect lines shows grain misorientation and increased material strength under applied strain.

Figure 8 also shows that increasing deformation in the materials increases both the number of dislocations and their total length. Figures 7 and 8 offer deeper insights into the plastic deformation mechanisms of Cu-Ta FGM at the atomic scale. In the plastic range, the number of grains decreases, and grain growth begins.

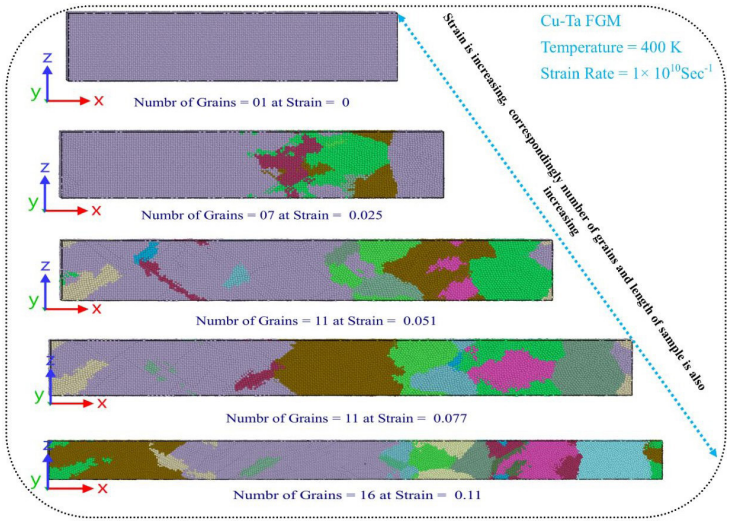



**Figure 9.** Grain segmentation of Cu-Ta FGM structure at fixed strain rate $1 \times 10^{10}$ $sec^{-1}$ and fixed temperature 400 K

Figure 9 illustrates the variation in grain size and the number of grains. Grain segmentation was used to find and separate grains with different orientations after the application of strain. As shown in Figure 9, at the first strain level there was no change in the crystalline structure; the previously selected monocrystalline structure was seen up to 0.025% strain. As the strain increased to 0.025%, 0.051%, 0.077%, and 0.11%, the monocrystalline structure gradually transformed into a polycrystalline structure, with the number of grains increasing to 7, 11, 11, and 16, respectively. The Cu-Ta interfacial region plays a significant role in controlling the deformation behavior of the FGM due to the mismatch between the FCC Cu and the BCC Ta crystal structures. During tensile loading, the interface acts as a barrier to dislocation propagation, resulting in localized stress accumulation and enhanced strengthening. The graded compositional transition eases progressive load transfer across phases, thereby minimizing abrupt interfacial stress concentration. At elevated temperatures, increased atomic diffusion and increased dislocation mobility near the interface contribute to defect redistribution and to the thermodynamic stabilization of the material. The present MD results show good agreement with earlier studies on Cu-based systems, particularly in terms of elastic modulus, yield strength, and diffusion coefficients at elevated temperatures. The observed deformation mechanisms, such as dislocation nucleation and grain boundary sliding, are also consistent with prior atomistic simulations. This is essential for understanding microstructural properties and their influence on material behavior.

### 3.2. Mechanical properties variation with temperatures at fixed strain of $1 \times 10^9$ $sec^{-1}$

Figure 10, depicts the variation of temperature with fixed strain rate at $1 \times 10^9$ $sec^{-1}$, with the interval of 200 K temperatures ranges from 200 K to 1000 K.

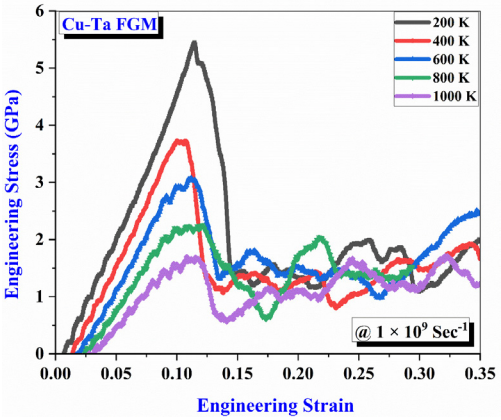



**Figure 10.** Engineering stress and engineering strain with fixed strain rate $1 \times 10^9$ $sec^{-1}$

Figure 10 shows that, as temperature increases, the graph shifts downward. It is concluded that the highest strength is obtained at the lowest temperature 200 K; with further increases in temperature, the highest point on each graph moves downward almost linearly at a constant strain level. The increase in strength is associated with dislocation density, sharp changes in structure, and more grain boundaries.

## 4. Conclusion

MD simulations of Cu-Ta FGM at four strain rates and five temperatures were performed using the EAM method. It provides a comprehensive analysis of mechanical property dependencies, microstructural changes, yield strength, and ultimate tensile strength. The following observation was made in the present study:

1. By increasing strain rate the material deformation mechanism changes due to less time for deformation and results in rapid fracture of Cu-Ta FGM without much deformation.
2. At higher temperatures, material behavior differs from that at low temperatures changes in deformation mechanisms.
3. As strain increases, the number of grains initially increases due to grain boundary strengthening after a critical value is reached, it decreases due to grain growth and elongation in Cu-Ta FGM.
4. The Response time of Cu-Ta FGM at higher strain

rates decreases due to sudden changes in the material's mechanical properties.
5. Mechanical strength, Youngs modulus decreases with increasing temperatures due to less bond strength
6. Cu-Ta FGM is suitable candidates at medium strain rate and lower temperature application.

## Author contributions statement

Dhowmya Bhatt: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Visualization, Writing – Original Draft Preparation., Nagajyothi Koripella: Supervision, Validation, Writing – Review & Editing, Project administration.

## Declaration of interests

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

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

## Declaration of generative AI and AI-assisted technologies in the writing process

The authors declare that no generative AI or AI-assisted technologies were used in the writing, preparation, analysis, or editing of this manuscript.

## Copyright permission

Figure 3 has been reproduced from [44] with permission from the respective authors and copyright holder.

## References

[1] Miyamoto, W. a. Kaysser, B. H. Rabin, A. Kawasaki, and R. G. Ford, Functionally Graded Materials: Design, Processing and Application. 1999.

[2] Finot and S. Suresh, "Small and large deformation of thick and thin-film multi-layers: Effects of layer geometry, plasticity and compositional gradients," J. Mech. Phys. Solids, vol. 44, no. 5, pp. 683–721, May 1996, doi: 10.1016/0022-5096(96)84548-0.

[3] Li and B. Han, "Research and Application of Functionally Gradient Materials," in IOP Conference Series: Materials Science and Engineering, Aug. 2018, vol. 394, no. 2, doi: 10.1088/1757-899X/394/2/022065.

[4] Miyamoto, "The applications of functionally graded materials in Japan," Mater. Technol., vol. 11, no. 6, 1996, doi: 10.1080/10667857.1996.11752708.

[5] Liu, F. Yuan, and Y. Wei, "Grain size effect on the hardness of nanocrystal measured by the nanosize indenter," Appl. Surf. Sci., vol. 279, pp. 159–166, Aug. 2013, doi: 10.1016/j.apsusc.2013.04.062.

[6] Li et al., "On the role of weak interface in crack blunting process in nanoscale layered composites," Appl. Surf. Sci., vol. 433, pp. 957–962, Mar. 2018, doi: 10.1016/j.apsusc.2017.10.002.

[7] Inoue, S. Nambu, Y. Ishimoto, and T. Koseki, "Fracture elongation of brittle/ductile multilayered steel composites with a strong interface," Scr. Mater., vol. 59, no. 10, pp. 1055–1058, Nov. 2008, doi: 10.1016/J.SCRIPTAMAT.2008.07.020.

[8] Cui, J. et al. Antibacterial activity, corrosion resistance and wear behavior of spark plasma sintered Ta-5Cu alloy for biomedical applications. J. Mech. Behav. Biomed. Mater. 74, 315–323. https://doi.org/10.1016/j.jmbbm.2017.06.022 (2017).

[9] Shen, Q. et al. Advances in copper-based biomaterials with antibacterial and osteogenic properties for bone tissue engineering. Front. Bioeng. Biotechnol. 9, 1526. https://doi.org/10.3389/fioe.2021.795425 (2022).

[10] Liang, D. et al. Fabrication of porous tantalum with low elastic modulus and tunable pore size for bone repair. ACS Biomater. Sci. Eng. 9, 1720–1728. https://doi.org/10.1021/acsbiomaterials.2c01239 (2023).

[11] Fraser, D., Funkenbusch, P., Ercoli, C. & Meirelles, L. Biomechanical analysis of the osseointegration of porous tantalum implants. J. Prosthet. Dent. 123, 811–820. https://doi.org/10.1016/j.prosdent.2019.09.014 (2020).

[12] Wang, H. et al. Comparison of 3D-printed porous tantalum and titanium scafolds on osteointegration and osteogenesis. Mater. Sci. Eng. C 104, 109908. https://doi.org/10.1016/j.msec.2019.109908 (2019).

[13] Liverani, E. et al. Mechanical interaction between additive-manufactured metal lattice structures and bone in compression: implications for stress shielding of orthopaedic implants. J. Mech. Behav. Biomed. Mater. 121, 104608. https://doi.org/10.1016/j.jmbbm. 2021.104608 (2021).

[14] Gupta, M. K., Rai, S. K., Panwar, V., Mahapatra, R. P., & Tevatia, A. (2026). Effect of nanoalloying on dynamic thermophysical response of polycrystalline copper-tantalum. Journal of Molecular Modeling, 32(3), 57.

[15] Gupta, M. K., Panwar, V., & Mahapatra, R. P. (2023). Effect of temperature and strain rate on mechanical properties and potential energy of nanocrystalline tantalum. Materials Today: Proceedings, 82, 22-28.

[16] Gupta, M. K., Mahapatra, R. P., & Panwar, V. (2022). Effect of Temperature and Strain Rate Variation on Tensile Properties of a Defective Nanocrystalline Copper-Tantalum Alloy. Journal of Scientific & Industrial Research, 81(04), 358-366.

[17] Korabi, R., Shemtov-Yona, K., Dorogoy, A. & Rittel, D. Te failure envelope concept applied to the bone-dental implant system. Sci. Rep. 7, 2051. https://doi.org/10.1038/s41598-017-02282-2 (2017).

[18] Lee, S. et al. Deformation, dislocation evolution and the non-Schmid efect in body-centered-cubic single- and polycrystal tantalum. Int. J. Plast. 163, 103529. https://doi.org/10.1016/j.ijplas.2023.103529 (2023).

[19] Chen, J., Mathaudhu, S. N., Tadhani, N. & Dongare, A. M. Unraveling the role of interfaces on the spall failure of Cu/Ta multilayered systems. Sci. Rep. 10, 208. https://doi.org/10.1038/s41598-019-57048-9 (2020).

[20] Maheshwari, S. U., Solomon, A. B., Thilagavathi, G., Hemamalin, M., & Illakkiam, D. (2025). Highly viable nanoparticle based Thermal Interface Materials (TIM) for electronics device cooling applications. Journal of Thermal Engineering, 11(5), 1312-1326.

[21] Jayaprakash, V., Ganesan, S., Beemkumar, N., & Sunil Kumar, M. Analysis of energy and exergy of a thermal storage system using multiple phase change material. Journal of Thermal Engineering, 11(4), 1160-1175.

[22] Muniamuthu, S., Kumar, K.S., Raja, K. and Rupesh, P.L., 2022. Dynamic characterization of hybrid composite based on flax-/E-glass epoxy composite plates. Materials Today: Proceedings, 59, pp.1786-1791.

[23] Kumar, K.S., Srinivasan, R.G., Palani, S., Čep, R., Salunkhe, S. and Nasr, E.A., 2025. Mechanical characterization of sisal fiber-groundnut shell powder reinforced epoxy composites. Scientific Reports, 15(1), p.33149.

[24] Muniamuthu, S., Raju, N.L., Sathishkumar, S. and Kumar, K.S., 2016. Investigation on mechanical properties of Al 7075-Al2O3 metal matrix composite. International Journal of Mechanical Engineering and Technology, 7(6), pp.474-482.

[25] Sunil Kumar, K., Muniamuthu, S. and Tharanisrisakthi, B.T., 2022. An investigation to estimate the maximum yielding capability of power for mini venturi wind turbine. Ecological Engineering & Environmental Technology, 23.

[26] Kumar, K.S., Kalos, P.S., Akhtar, M.N., Shaik, S., Sundara, V., Fayaz, H., Khan, S.A. and Asif, M., 2023. Experimental and theoretical analysis of exhaust manifold by uncoated and coated ceramics (Al2O3, TiO2 and ZrO2). Case Studies in Thermal Engineering, 50, p.103465.

[27] Gupta, M. K., Panwar, V., & Mahapatra, R. P. (2022). Computational analysis of mechanical behavior and potential energy of thermoresponsive copper-tantalum nanoalloy. Journal of Molecular Modeling, 28(7), 187. https://doi.org/10.1007/s00894-022-05183-y

[28] Zhou, Q. et al. Strain rate sensitivity of Cu/Ta multilayered flms: Comparison between grain boundary and heterophase interface. Scripta Mater. 111, 123–126. https://doi.org/10.1016/j.scriptamat.2015.08.031 (2016).

[29] Remington, T. P. et al. Spall strength dependence on grain size and strain rate in tantalum. Acta Mater. 158, 313–329. https://doi.org/10.1016/j.actamat.2018.07.048 (2018).

[30] Gupta, M.K., Guha, S., Singh, N.P. et al. Computational Analysis of Gold–Platinum Nanowires Subjected to Uniaxial Tensile Loading. J. Inst. Eng. India Ser. D (2024). https://doi.org/10.1007/s40033-024-00836-z

[31] Gupta, M. K., Rai, S. K., Panwar, V., Parinov, I. A., & Haldkar, R. K. (2023, October). Molecular Dynamic Study of Dependency on Mechanical Characteristic of Nanocrystalline Copper over Various Temperature and Strain Rate. In International Conference on Physics and Mechanics of New Materials and Their Applications (pp. 345-354). Cham: Springer Nature Switzerland.

[32] Pan, Z., Li, Y. & Wei, Q.(2008) Tensile properties of nanocrystalline tantalum from molecular dynamics simulations. Acta Mater. 56, 3470–3480. https://doi.org/10.1016/j.actamat.2008.03.025 .

[33] Hahn, E. N., Germann, T. C., Ravelo, R., Hammerberg, J. E. & Meyers, M. A. On the ultimate tensile strength of tantalum. ActaMater. 126, 313–328. https://doi.org/10.1016/j.actamat.2016.12.033 (2017).

[34] Mebarek-Oudina, Fateh, and I. Chabani. "Review on nano-fluids applications and heat transfer enhancement techniques in different enclosures." Journal of Nanofluids 11.2 (2022): 155-168.

[35] Mebarek-Oudina, F., & Chabani, I. (2023). Review on nano enhanced PCMs: insight on nePCM application in thermal management/storage systems. Energies, 16(3), 1066. https://doi.org/10.3390/en16031066

[36] Mebarek-Oudina, F., Bouselsal, M., Khan, S. U., Ramesh, K., & Ismail, A. I. (2025). Optimizing thermal performance in shell-and-tube heat exchangers with tri-hybridised nanofluids: a numerical study of turbulent convection. Thermal Science and Engineering Progress, DOI 10.1016/j.tsep.2025.103988

[37] Naseem, T., Mebarek-Oudina, F., Shahzad, A., Fish, H., & Hamida, M. B. (2026). Enhanced thermodynamic irreversibility and heat transfer in rotating graphene oxide–water nanofluids over a stretching surface. Modern Physics Letters B, 40(03), 2550267. https://doi.org/10.1142/S0217984925502677

[38] Zhou, R.A. Johnson, and H.N.G. Wadley (2004), "Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers", Physical Review B, 69(14), 144113. DOI: 10.1103/physrevb.69.144113.

[39] Plimpton, "Fast parallel algorithms for short-range molecular dynamics," J. Comput. Phys., vol. 117, no. 1, pp. 1–19, Mar. 1995. DOI 10.1006/jcph.1995.1039

[40] Stukowski, "Visualization and analysis of atomistic simulation data with OVITO—The open visualization tool," Model. Simul. Mater. Sci. Eng., vol. 18, no. 1, Jan. 2010, Art. no. 015012. DOI 10.1088/0965-0393/18/1/015012

[41] Falco, S., Jiang, J., De Cola, F. & Petrinic, N. Generation of 3D polycrystalline microstructures with a conditioned Laguerre-Voronoi tessellation technique. Comput. Mater. Sci. 136, 20–28. https://doi.org/10.1016/j.commatsci.2017.04.018 (2017).

[42] Larsen, P. M., Schmidt, S. & Schiøtz, J. Robust structural identifcation via polyhedral template matching. Modell. Simul. Mater.Sci. Eng. 24, 055007. https://doi.org/10.1088/0965-0393/24/5/055007 (2016).

[43] Kelchner, C. L., Plimpton, S. J. & Hamilton, J. C. Dislocation nucleation and defect structure during surface indentation. Phys. Rev.B 58, 11085–11088. https://doi.org/10.1103/PhysRevB.58.11085 (1998).
[44] Gupta, M. K., Mahapatra, R. P., & Panwar, V. (2022). Effect of temperature and strain rate variation on tensile properties of a defective nanocrystalline copper-tantalum alloy. J. Sci. Ind. Res, 81, 358-366.