



Effect of Temperature and Strain Rate Variation on Tensile Properties of a Defective Nanocrystalline Copper-Tantalum Alloy

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Nanocrystalline alloys of immiscible in nature are emerging topics of interest for researchers due to better mechanical stability at high temperatures. Nanocrystalline Copper-Tantalum alloy is of particular interest for research exploration due to its high strength, limited solubility and high-temperature stability. In the present work, the mechanical properties of nanocrystalline 90/10 copper-tantalum (9Cu-Ta) alloy have been investigated using the molecular dynamics approach. Embedded atom method (EAM) of potential has been used to analyze the mechanical properties at high temperatures due to the high stability of EAM in molecular dynamic simulation. At high-temperature defects plays a very important role therefore a specific 9Cu-Ta nanostructure having 3% vacancies has been selected to explore its performance under a particular type of point defect. This study has been conducted under uniaxial tensile loading. The tensile properties of this defective nanocrystalline alloy have been compared at specific temperatures i.e. 300 K, 600 K, 800 K, 1000 K and 1200 K. The study revealed that the variation in temperature from 300 K to 1200 K results in the shifting of the stress-strain graph to lower stress values. It has also been noticed that the variation in ultimate tensile strength is the least in comparison to yield strength and elastic constant for the same variation in temperature. These results indicate the importance of avoiding thermal agitations during the synthesis and surface modification of nanocrystalline copper-tantalum alloy.

Keywords: Mechanical properties, Modeling and simulation, Molecular dynamics, Point defect, Vacancy

Introduction

During the past few years, it is of great interest to find the material has a high strength to weight ratio. The theoretical determination of mechanical properties of metallic materials is now-a-days having great importance as compared to the experimental determination of properties of metallic materials. The material properties such as yield strength, ductility and elasticity of metals are highly affected by the working pressure. In the case of the single crystal when the deformation exceeds the elastic limit, a plastic flow occurs due to the generation of the defect. The rearrangement of atoms from their current position describes the plasticity of atoms at the atomic scale. Generally, the structure models in civil engineering, mechanical engineering as well as in material science use stress which is the major component to measure the plastic deformation and strength of material.¹

Copper (Cu) is a transition metal that is known for its high electric and thermal conductivity along with

being a soft, malleable and ductile element. Cu is known to form alloys more freely than other metals. The same cannot be concluded when considering a refractory metal such as Tantalum (Ta) which is known for its high corrosion resistance and biocompatibility apart from being a lustrous and hard transition metal. Copper-Tantalum (Cu-Ta) alloys present themselves as an immiscible system.² Nanocrystalline material with its great difference in electronegativities of Cu and Ta suggests the formation of an intermetallic compound of these elements. In the present study, the composition of Cu and Ta for the alloy is 9/1, as per atomic weight. This atomic weight composition is chosen as per the experimental observation made while inventing Cu-Ta alloy, which states that mostly Cu-Ta alloys can be prepared with a maximum of 50 wt% of Ta, and further even at 1200°C only 0.009% atoms of Ta are soluble in Cu. It has been observed that Cu-Ta offers strong resistance against grain growth proving them to have high thermal stability and mechanical strength, especially at elevated temperatures.³ The stability in mechanical properties of Cu-Ta nanocrystalline alloy

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is attributed to the presence of Ta atoms along the grain boundaries as well as dislocations within the grains. Herein, the presence of dislocations is responsible for the stability and strength of the crystal. As per the study conducted by Li *et al.* for α -Zr, vacancies slightly affect the stress-strain curves and do not change the shape of the curves, further claiming that even Young's modulus remains equal.⁴ Nevertheless, this claim is not in agreement with Zhu *et al.*, where the observation for Young's modulus is the decrease in its value with an increase in vacancy concentration for Zr.⁵ Though stress is a major parameter for quantifying plastic deformation but the existence of interfaces in nanocrystal also contributes for an increase in the plasticity of the material.⁶ It can be noticed that the elastic modulus of single as well as in polycrystalline tantalum alloys decreases with increasing temperature.⁷ The strain rate dependence on the strength of nanocrystalline metal becomes stronger for metals having face-centered cubic (FCC) structure and weaker for body-centered cubic (BCC) structured metals. Since Cu is FCC and Ta is BCC in structure so the concept of strain dependence cannot be particularly defined for Cu-Ta alloys.⁸ According to Tang *et al.*, BCC metals show an asymmetry in flow stress due to the core effects related to dislocations.⁹ Nanocrystalline Cu-Ta alloys are most popularly used in nano- and micro-electronics applications wherein Ta mainly acts as a diffusion barrier. Targeted applications of Cu-Ta alloys are based on the requirements of typical component usage under special conditions of high temperature, strength and/or oxidation-resistant properties.

This paper aims to study the stability of mechanical properties of nanocrystalline 9Cu-Ta alloy at discrete strain rates ranging between 1×10^8 /sec to 8×10^{10} /sec. In addition, it is also focused to observe the changes in mechanical properties of 9Cu-Ta nanoalloy under the influence of 3% vacancy at discrete temperatures ranging from 300 to 1200 K at a fixed strain rate of 5×10^{10} /sec.

Methodology used for Simulation Technique

The classical molecular dynamics simulation approach has been used to conduct this study. Molecular dynamics (MD) is a computational tool for simulating both the solid and liquid molecules where each of the N atoms is treated as a point mass and their integrated motions are further computed using Newton's equation. For applying this MD simulation,

an open-access software LAMMPS has been used.¹¹ Velocity verlet algorithm has been used to solve Newton's equation. One of the reasons to use classical molecular dynamics is due to the advantage of molecular dynamics over the ab initio electronic calculations of describing the dynamic behavior of atoms without having to solve Schrodinger's equation. In fact, molecular dynamics tend to describe the atomic interaction using classical mechanics and hence well suited to simulate the structure and mechanical properties in nanoscales. Especially, molecular dynamic simulation is quite effective in studying the mechanics of defects and their interaction in an environment of a large number of free surfaces in nanostructures.¹² Furthermore, Ab initio technique tends to show a certain deficiency in describing point defects.¹³ Therefore, to overcome these disadvantages of ab initio and since this study also incorporates vacancy defect, MD simulation in LAMMPS with the interatomic potential of Embedded Atomic Model (EAM) is considered. EAM potential is well suited to requirements of creating point defects such as vacancy defects. Additionally, since EAM is a density-dependent energy function it gives an advantage of defined electron density, unlike the pair potential which are volume-dependent energy¹⁴ and as opposed to EAM neglect many-atom interaction.¹⁵ While force fields are important to create an accurate interatomic potential within the system, it is equally important to define the boundary conditions to approximate a large system into smaller parts called a unit cell. In this study, the boundary conditions follow the periodic order and the simulation box is in cubic form. The reason to choose this specification is that the alloy is a cubic crystal and also because ordered phase crystals need to accommodate a substantial number of crystals unit cells.¹⁶ To visualize the behavior of material OVITO software tool has been used.¹⁷ In order to obtain accurate values of velocities the algorithm utilizes the positions $r(t)$, velocities $v(t)$, and accelerations $a(t)$, at the same time

$$r(t + \Delta t) = r(t) + v(t)\Delta t + \frac{[a(t)(\Delta t)^2]}{2} \quad \dots (1)$$

$$v(t + \Delta t) = v(t) + \frac{\Delta t[a(t) + a(t + \Delta t)]}{2} \quad \dots (2)$$

The above equations are implemented in two steps. First, the positions and velocities at time step $(t + \Delta t)$

are calculated with the help of Eqs (1) & (2), respectively. Velocities at mid-step are calculated using Eq. (3) which is given as,

$$v\left(t + \frac{\Delta t}{2}\right) = v(t) + \frac{[a(t)]\Delta t}{2} \quad \dots (3)$$

Then the accelerations at time $(t + \Delta t)$ are computed and thus velocity is calculated using Eq. 4 which is given as,

$$v(t + \Delta t) = v\left(t + \frac{\Delta t}{2}\right) + \frac{[a(t + \Delta t)]\Delta t}{2} \quad \dots (4)$$

Using Eq. (4), the kinetic energy (KE) is obtained at different time steps. The relation of KE with velocity and temperature, respectively are represented by Eqs (5) & (6).

$$KE = \frac{mv^2}{2} \quad \dots (5)$$

$$KE = \frac{3}{2}kT \quad \dots (6)$$

Using Eqs (5) & (6), the relation between absolute temperature and the velocity of atoms/molecules can be given as shown in Eq. (7),

$$T \propto v^2 \quad \dots (7)$$

The analysis has been performed on the crystal lattice of the nanocrystalline alloy arranged in an orthogonal space. The parameters at which the simulation has been carried out are given in Table 1.

The crystal is formed with the help of ATOMSK (open-source software maintained by Pierre Hirel at the university of Lille, sciences and technologies) software by taking copper and tantalum atoms.¹⁸

Table 1 — Typical parameters used for the simulation of 9Cu-Ta

Parameters	Values
Temperatures (K)	300, 600, 800, 1000 and 1200
Strain rates (per second)	1.0×10^8 /sec, 1.0×10^9 /sec, 1.0×10^{10} /sec, 5.0×10^{10} /sec, and 8.0×10^{10} /sec
Simulation time step (picoseconds)	0.001
Vacancy concentration	3%

Simulation has been employed using LAMMPS software, the simulation was started with 9Cu-Ta alloy. To achieve the lattice parameter was set for the alloy which fixed the dimensions of the unit cell to give it a form of the crystal under study. For creating the alloy of Cu-Ta in the simulation the lattice constant of both Cu as 3.61 Å and Ta as 3.30 Å were considered as taken to the experiments.^{19,20} While performing the simulation it was made sure that there is minimum possible angular and linear momentum along with lesser vibration between atoms in the system to create vacancy and deformation which could be further studied keeping aside other unwanted factors such as oscillation and collisions between the atoms of the system, and therefore a drag coefficient of 1 was provided. To provide a real environment, a practical dimension was given to the simulation box of $53.95 \times 53.95 \times 53.95$ while creating the periodic boundary conditions. This dimension of the simulation box helped to create a total number of 13500 atoms of which 12150 were copper and 1350 were tantalum. In order to obtain an accurate and precise result, apart from providing a practical environment, utmost priority was given to the systems or the atoms interacting within to reach the point of equilibrium. Through energy minimization, stable conformations can be identified which in turn gives a state where atomic forces become zero²¹, which can be observed from Fig. 1 (a & b), which shows the crystal before and after energy minimization effect on the nanocrystalline alloy. In the study, the atoms to achieve their point of stabilization stated the stopping energy and force tolerance where the iterations would stop and relax. The minimization has been performed as per the Polak-Riberia conjugate gradient (CG) algorithm²² which has been described that CG algorithm at every iteration, the force gradient is combined with the previous iteration to compute a new search direction perpendicular to the previous one.^{23,24} Therefore, the directions are specified after each step of the iteration.²⁵ A time step of 0.001 picoseconds is set for the equilibration.

For providing the design constraints to the system of atoms, an isothermal-isobaric ensemble (NPT) ensemble has been selected. An NPT ensemble is a system of the constant number of atoms along with constant temperature and pressure. The motive of using this ensemble is to set the desired temperature and pressure for analyzing the effect of subsequent

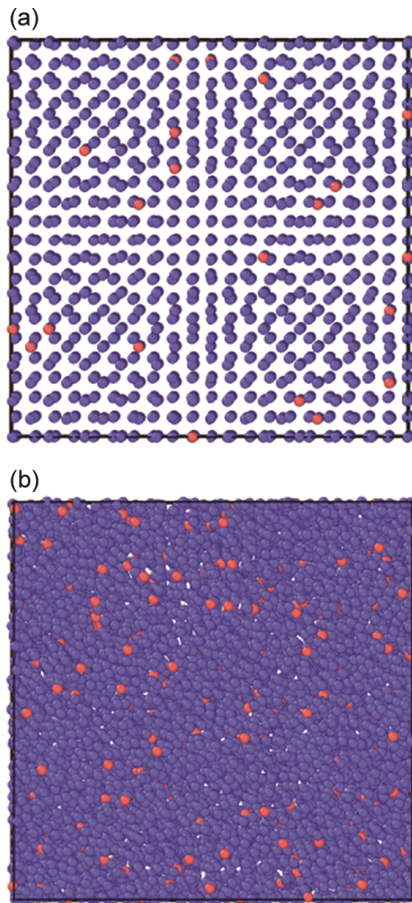


Fig. 1 — Visualization of 9Cu-Ta (a) before energy minimization, (b) after energy minimization

parameters on the modelled structure before and after the deformation of the structure, as shown in Fig. 2 (a – f). At the same moment, it allows the energy and enthalpy²⁶ to fluctuate according to the artificial environment, revealing the energy and other mechanical properties (e.g. stress and strain) at the point of equilibrium in all the desirable directions.

The model under canonical Number of atoms-Volume- Temperature ensemble (NVT) first relaxes for 1 femtosecond to reach an equilibrium state. Thereafter, the loading is applied under the isothermal-isobaric ensemble (NPT) using the Nose-Hoover method to control the temperature at a constant strain rate. The NPT ensemble is used to conserve pressure along with the number of particles and temperature. It is important to specify during MD simulation that there is a requirement of conservation of a number of particles to avoid any undefined loss of atoms. Subsequently, constant strain rates are provided to have equal continuous

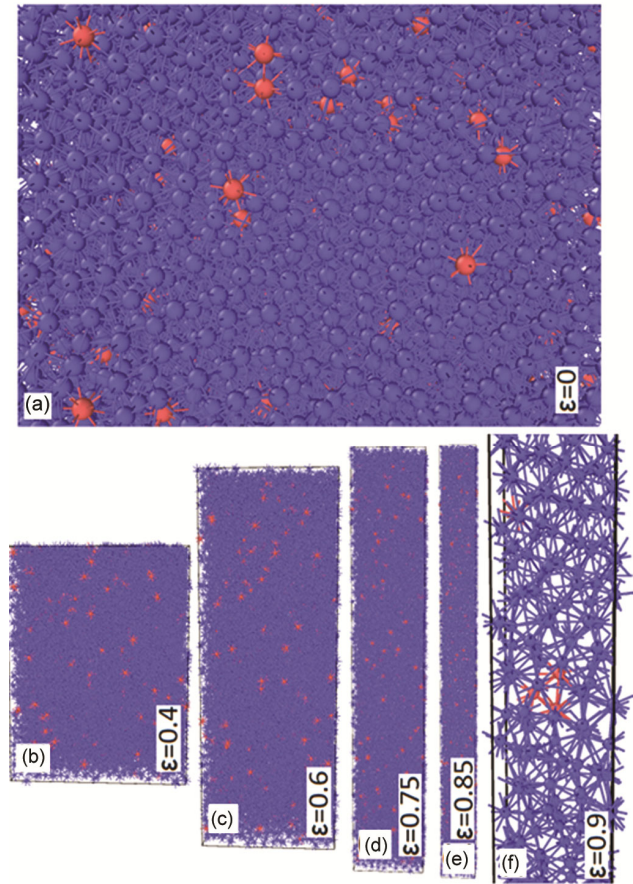


Fig. 2 — Structure of 9Cu-Ta: (a) after minimization but before deformation, (b – f) after deformation, at different levels of strain

deformation at different intervals of time. Therefore, with an increase in time, the longitudinal dimension of the box will increase, correspondingly its lateral dimension will decrease. It should be noted that these steps were taken to provide uniaxial tensile stress at five strain rates on a perfect crystal. Once deformation was performed, the simulation was again carried out but this time by creating a vacancy of 3%, deleting the required concentration from a group of atoms.

This led to the deletion of a total of 405 atoms with the final total being 13095 atoms. It should be noted that the defects are generated randomly throughout the material according to the given concentration. The program was developed to run the input script with the help of the software LAMMPS. In this consideration of 3% defects which removes 405 atoms from the given concentration of 9Cu-Ta. The output of the LAMMPS is obtained and analyzed the data in subsequent graphs and a dump file is used to visualize the defects with the help of OVITO software.

Results and Discussion

Effect of 3% Vacancy and Strain Rate at Room Temperature (i.e. 300 K)

The stress-strain behavior of nanocrystalline 9Cu-Ta has been shown in Fig. 3. Both the perfect and defective crystals depict a similar trend. However, the vacancy concentration induced leads to a huge drop in both the ultimate tensile and yield strengths of the material with percentage changes being 19.5% and 15.2% respectively. Young's modulus has also decreased by around 13% but the corresponding effect is less in comparison to the relative changes in tensile and yield strengths. Although, by looking at Table 2 it can be concluded that a similar trend is not followed by the material religiously at higher temperatures. This loss in strength and elastic modulus can be attributed to the irregular motion within the atoms in

their ability to reach the point of equilibrium or lower energy level. As we can conclude from Fig. 3, a deviation in graphs of perfect crystal and vacant crystal is due to the energy required to create the vacancy in the crystal. Vacancy formation energy is responsible for the decrement in the overall strength of the vacant crystal.

The simulation was performed for varying strain rates of the order of 1×10^8 /sec, 1×10^9 /sec, 1×10^{10} /sec, 5×10^{10} /sec, and 8×10^{10} /sec. at a constant temperature of 300 K. This was carried out for a perfect crystal, as can be seen from Fig. 4. It is quite clear that with an increase in the strain rate the area covered by the stress-strain graph also increases which indirectly increases the toughness. The overall property including the strength and Young's modulus

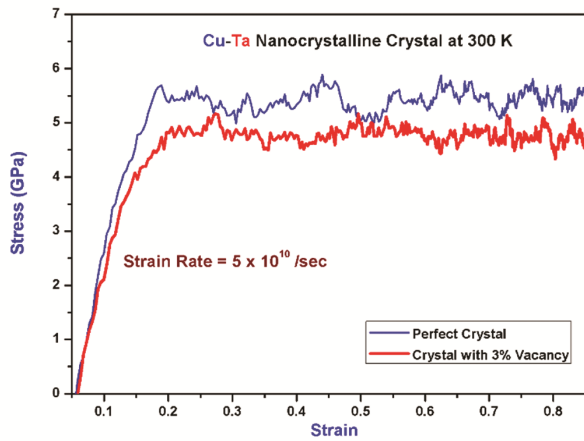


Fig. 3 — Stress-Strain curves for perfect and defective crystal at 300 K under the applied strain rate of 5×10^{10} /s

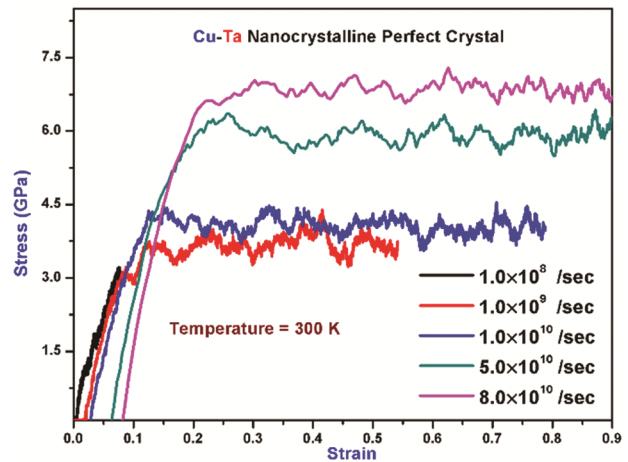


Fig. 4 — Stress-strain behaviour of 9Cu-Ta under the influence of different strain rates at fixed temperature

Table 2 — Effect of 3% vacancy in 9Cu-Ta alloy on selective mechanical properties at different temperatures

Temperature (K)	Crystal Type	Properties (GPa)		
		Yield Strength	Ultimate Strength	Young's Modulus
300	Perfect Crystal	5.66	7.27	31.12
	3% Vacancy	4.8	5.85	27.1
	% change (-ve)	15.2	19.5	12.9
600	Perfect Crystal	5.01	7.11	27.74
	3% Vacancy	4.43	5.52	26.52
	% change (-ve)	11.4	22.4	4.4
800	Perfect Crystal	4.83	7.03	26.59
	3% Vacancy	4.42	5.37	22.55
	% change (-ve)	8.5	23.6	15.2
1000	Perfect Crystal	4.25	6.03	24.1
	3% Vacancy	3.81	5.23	22.48
	% change (-ve)	10.3	13.3	6.7
1200	Perfect Crystal	3.14	5.58	22.14
	3% Vacancy	3.01	4.82	18.99
	% change (-ve)	4.1	13.6	14.2

of materials increases with increasing strain rates. The trend that we observed is similar to what we have in the case of lowering the value of temperature at a fixed strain rate. The effect displayed by the higher strain rate is somewhat similar to that with lower temperature, which increases and enhances the overall property and strength of the material. This is mainly because with a high strain rate the dislocation movement was given a shorter time to consume continuous work done by the surroundings²⁷, and hence the copper tantalum alloy is allowed to consume less energy by dislocation movement and it also prevents the alloy to reach in its equilibrium. Because of shorter duration is allowed at higher strain rates for dislocation movement which led to an increase in stress values.

Effect of Increasing Temperature on Stress-Strain Behavior

A stress-strain curve was obtained as output after the completion of the simulation. The variation of stress and strain at a constant strain rate of $5.0 \times 10^{10}/\text{sec}$ under varying temperatures of 300, 600, 800, 1000, and 1200 K for a perfect crystal and crystal with 3% vacancy are shown in Figs 5 & 6. According to the trend followed by the stress-strain curve, it can be concluded that alloy system under consideration is ductile in its nature, as the plastic deformation covers a substantial section of the curve and there is no sudden fracture when stress is applied beyond the elastic range or upper yield point. However, the obtained graph presents a bit of unusual behavior of copper tantalum alloy. According to Turnage *et al.*, it has been highlighted that the strength of copper tantalum alloy is high at elevated temperatures due to the property exhibited by tantalum nano-clusters of pinning the grain boundaries and dislocation motion.³ On the other hand, as per the observation from the simulation result in the present study, with the increase in temperature the toughness which is nothing but the area under the stress-strain curve, decreases, therefore leading to a conclusion that the material tends to lose its strength with increase in the temperature.

Nonetheless, the outcomes do prove that copper tantalum is an intermetallic compound not just as per Hume-Rothery rules but also due to the observation made through the curve obtained since it is the solid solutions that interact with dislocations and hence restrict their motion thereby increasing the stress. But these trends show that stress is substantially decreasing. Furthermore, if given a glance at both the

trends of perfect crystal and the one with 3% vacancy, it is quite clear that the creation of defect is further reducing its strength to even lower values than that of the perfect crystal.

Mechanical Properties of Perfect and Defective Crystal of 9Cu-Ta at Selected Temperatures

The change in yield strength with an increase in temperature can be observed from Fig. 7. For both the perfect crystal and vacancy concentrated crystal can be seen that as the temperature increases the difference between the yield strengths for both types of crystal decreases. There is also an overall decrease in yield strength while approaching elevated temperatures. Although the strength reduces its value gradually, however, between a temperature range of 600 – 800 K, for perfect crystal, there is just a 3.59% change and for vacancy concentrated crystal

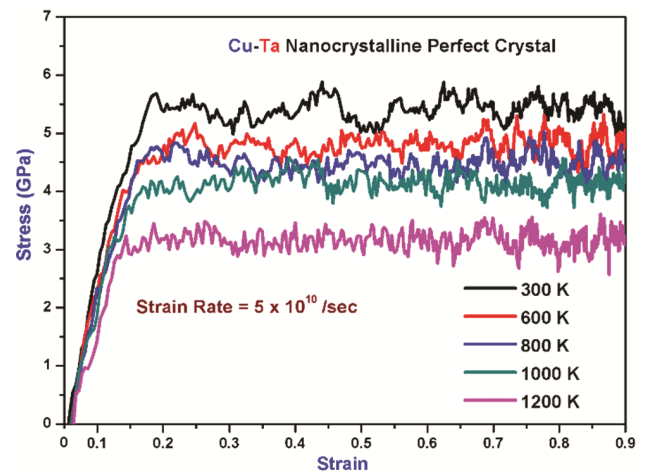


Fig. 5 — Influence of temperature on stress-strain response of perfect crystal of 9Cu-Ta

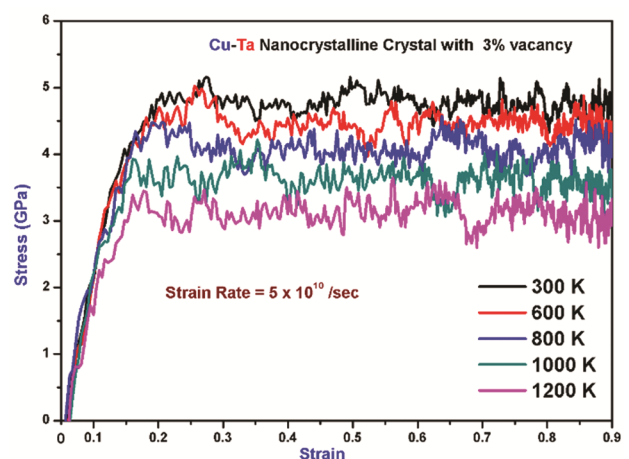


Fig. 6 — Influence of temperature on stress-strain response of 9Cu-Ta having 3% vacancy at fixed strain rate

the reduction is by a very minute percentage of 0.23%.

This means that the value somewhat remains constant for both the cases at 600 – 800 K and suddenly there comes a steep depletion in the value with approximately equal observed yield strength at 1200 K of 3.14 GPa and 3.01 GPa for perfect and imperfect crystals, respectively. It can be concluded that at higher temperatures, yield strength or the stress required to activate plastic deformation becomes nearly independent of vacancy concentration. The decrease in yield strength has been observed at higher temperatures which is due to the thermally activated dislocation within the crystal.²⁸ The close variation in the values of yield strength, ultimate tensile strength (UTS), and Young’s modulus

at various temperatures has been already shown in Table 2.

The relationship between Young’s modulus and temperature at a constant strain rate for both perfect and vacancy concentrated crystals has been shown in Fig. 8. As it has been previously elucidated that the area covered by the stress-strain curve decreases with the increase of temperature as well as with the imperfection induced in the crystal, and therefore Young’s modulus or the ability of the material to maintain its elasticity also decreases when a vacancy is created. In both cases, as the temperature increases the modulus decreases from 31.12 GPa to 22.14 GPa for perfect crystal and 27.09 GPa to 18.99 GPa for vacancy concentrated crystal. This is due to the increase in vibration amongst the atoms which further leads to an increase in their atomic distance and depletion of interatomic forces. In case of vacancy creation, the atoms start vibrating even more energetically with the removal of atoms and therefore the rate of increase in their atomic distance becomes higher. The same can be observed from the graph between Young’s modulus and temperature, that for a perfect crystal the decrease is a gradual one, however, for the crystal with 3% vacancy, there is a sudden and steep decline in the values between 600 – 800 K and 1000 – 1200 K.

The ultimate tensile strength of the material which provides the value of maximum strength that material possesses after the strain hardening and just before necking also decreases with both the increase in temperature and vacancy concentration as can be seen in Fig. 9. However, as can be observed from the graph

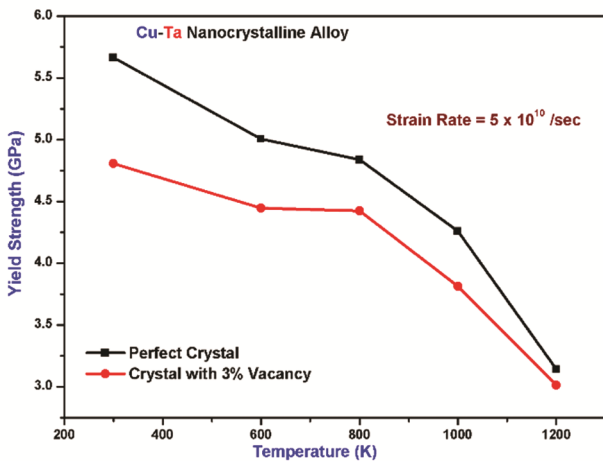


Fig. 7 — Yield strength of perfect and defective crystals of 9Cu-Ta at fixed strain rate

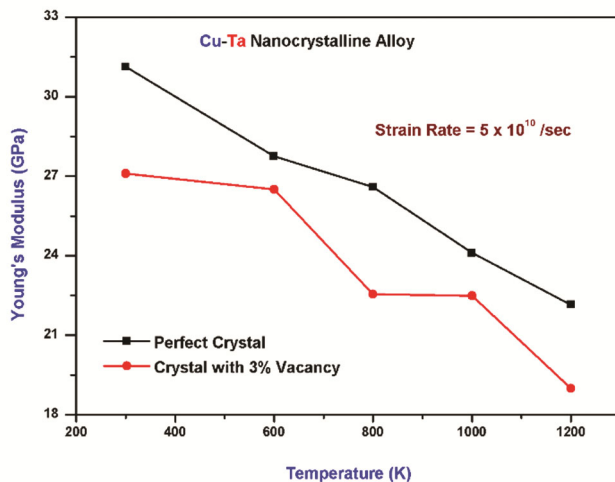


Fig. 8 — Young’s modulus of perfect and defective crystals of 9Cu-Ta at a fixed strain rate and increasing temperatures

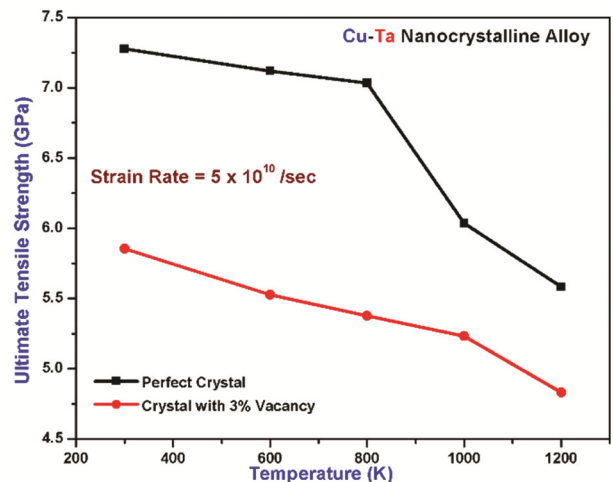


Fig. 9 — Ultimate tesile strength of perfect and defective crystals of 9Cu-Ta at increasing temperatures

that at lower temperatures the ultimate tensile strength gets more affected by crystal structure and distortions within it as compared to the temperature, since the observed decrease is by 19.5% at just 300 K from a perfect to imperfect distortion of crystal. The reduction in tensile strength of crystal, with temperature, having 3% vacancy is comparatively less than that of a perfect crystal. For the perfect crystal especially in the temperature range of 800 – 1000 K, there is a sudden drop by 14.20% in the tensile strength.

It seems that the material goes through some microstructural transformation within this temperature range but again after this temperature the strength decreases steadily. Overall, the decrease in strength is way more uniform in the case of a crystal with 3% vacancy than that of a perfect crystal. Further, it can be concluded that as the temperature rises material loses its ability to elongate and becomes a bit brittle in nature, thereby deviating from its ductile behavior at lower temperatures.

Conclusions

In the present study, stress-strain analysis of 9Cu-Ta has been conducted under different strain rates at a fixed temperature for a perfect crystal and under different temperatures ranging from low to elevated temperatures with perfect as well as 3% vacant crystal at a fixed strain rate, using molecular dynamic simulation approach. Ultimate tensile strength of perfect crystal decreases from 7.27 GPa to 5.58 GPa (i.e. 23%) with the increase in temperature from 300 to 1200 K, while for the crystals having 3% vacancy the corresponding reduction in tensile strength is around 17%. This shows the high sensitivity of vacancies for a decrease in tensile strength at near room temperature applications. A variation from considered room temperature to 1200 K shows a reduction in Young's modulus by 29% and 30%, respectively. These results explore the microstructural and mechanical stability of a nanocrystalline Cu-Ta alloy at higher temperatures which is a key concern while using it in typical applications related to nuclear energy, space industry, and transportation.

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