Irradiation studies on nano-scale single crystal copper by molecular dynamics simulation

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Abstract: We report molecular dynamics (MD) simulation studies on the structure and tensile properties (temperature =300 K and strain rate= 1010 s-1) of irradiated copper single crystals (101.8 Å × 50.54Å × 50.54 Å) oriented along the [100] and [110] crystallographic orientations. Primary knock-on atom (PKA) method is used for radiation (0.5 keV to 5 keV). Structural studies indicate liquid like regions near the PKA region and are more in [110] orientation. The self-diffusivity (D) of copper in the PKA regions is found to increase from 4.05 × 10−5 m2/s at 1 keV irradiation energy to 27.36 × 10−5 at 5 keV irradiation energy in [110] orientation. However, no such relationship is observed in the [100] orientation. Vacancies, self-interstitials, and dislocations are more prominent in [100] orientation (dislocation density = 1 × 1016 m−2). Young's modulus and yield strength decrease due to the formation of defects as anticipated.

1. Introduction
Radiation damage in copper single crystals has been extensively studied in the past[1]–[3]. Irradiation causes hardening of copper single crystal and is attributed to the dislocation locking as shown in the studies of Blewitt et al. [1]. Greenfield and Wilsdorf [2] have studied neutron irradiation effects on the plastic deformation of copper single crystal. They observed an increase in yield stress of irradiated sample and proposed that interaction between prismatic dislocation loops (resulting from coalescence of vacancies) and glide dislocations is the reason for such increase. Sood and Dearnaly [3] have found that there has been no significant surface damage on <110> oriented copper single crystal upon ion irradiation by Mo, Au, and Cu ions, rather, the damage has been extended to larger depths. The above studies indicate that radiation has a significant effect on the structural and mechanical properties of single crystals. However, none of the above studies reported the initial condition of the sample, i.e., whether perfect/defect by showing the concentration of vacancies or dislocations that could play an important role in the evolution of defect density, deformation mechanisms and hence the mechanical properties after irradiation. Furthermore, the microstructural changes observed in the samples are after irradiation mostly spanning from weeks to years. However, the primary irradiation damage corresponding to microstructural changes lasts for only a few picoseconds. To study the irradiation effects experimentally at such small time scales is a limitation. So, Molecular dynamics (MD) simulations have emerged as a powerful computational tool to study the irradiation damage at such spatial and small time scales[4]–[8]. Li et al. [5] studied ion irradiation induced defects on the mechanical properties of copper nanowires (NWs) from MD simulations. It is reported in the above study that radiation induces point defects and stacking faults (reported for the first time) in copper and lowers Young’s modulus. Using primaryknock-on atom (PKA) method with energy up to 20 keV, Korchuganov et al. [6] investigated the radiation damage in Fe-Cr alloy
crystallites. They observed vacancy type dislocation loops and the size of the defect clusters increased with PKA energy. Similarly, Buchan et al. [7] investigated radiation damage in adiamond with PKA energies up to 2.5 keV and observed only isolated point defects in the diamond samples. Furthermore, Jiang et al. [8] investigated through ab-initio MD simulations the effect of stacking faults on the radiation response of cubic SiC. They observed that stacking faults act as obstacles to the movement of C and Si atoms and promote radiation tolerance.

To date, extensive studies involving experimental and MD have been devoted to investigating radiation damage in single crystals[1]–[3], [5], alloys [6], [8], and interaction of pre-existing defects with radiation-induced defects [8] by ion irradiation or PKA method. Nevertheless, there are seldom studies reported on the combined effect crystal orientation and radiation damage. In this work, we carry out MD simulations to study the structure and tensile properties of irradiated copper single crystals oriented along the [100] and [110] crystallographic orientations. We have first investigated the stress-strain response and mechanical properties of pristine samples, and then simulated defect production (vacancies, interstitials, dislocations) induced by PKA method with different energies. Thereafter, we study the structural changes to identify amorphous/liquid like regions near the PKA region by radial distribution function (RDF) analysis. Also, we have tracked the atomic paths in these regions. Atomic mixing has been studied using mean square displacement analysis (MSD). Finally, we investigate the mechanical properties of the irradiated single crystals and evolution of dislocation density at different strains. These results may have practical implications in the prediction of performance and properties of materials for use in nuclear reactors.

2. Modeling and simulation details

![Atomic snapshot of copper single crystals](image)

**Figure 1.** (a, b) Atomic snapshot of copper single crystals of dimension 101.08 Å (x-axis) × 50.54 Å (y-axis) × 50.54 Å (z-axis) having different orientations a) [100]; b) [110]; c) sample showing the thermostat region, interior region and PKA atom; d) sample configuration for tensile deformation.

MD simulations on radiation damage and subsequent uniaxial tensile deformation have been carried out using Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [9]. Copper single crystal of dimension 101.08 Å (x-axis) × 50.54 Å (y-axis) × 50.54 Å (z-axis) (21952 atoms) as shown in Figure 1a and Figure 1b is constructed by filling the simulation box with copper atoms (FCC crystal structure and lattice constant a = 3.61 Å) in two different crystal orientations, i.e., [100] and [110] using periodic boundary conditions along the three directions. Wen et al. [10] used similar orientation Au nanowires to study the mechanical properties under uniaxial loading. Further, the size used in the present study is larger than that used in the irradiation studies on copper NWs (30 Å × 30 Å × 142.5 Å) conducted by Li et al.
[5]. EAM (Embedded Atom Method) alloy potential developed by Zhou et al. [11] which is implemented in LAMMPS is used for modeling the interaction between the Cu atoms during radiation damage and tensile deformation. This potential can well fit the basic material properties such as the lattice constant, the elastic constants, the bulk modulus, the sublimation energy, vacancy formation energy, and the heat of solution. Bukkuru et al. [12] used this potential for studying the self-interstitials in bcc and fcc crystals. Koch et al. [13] used this potential for irradiation damage studies in Cu based high entropy alloys. Furthermore, the potential has been used for studying the mechanical properties [14], [15]. Zhou et al. [14] studied the strain rate effect on the nano-crystalline copper. Zhang et al. [15] studied the grain size and shape on the mechanical properties of nanocrystalline copper.

Copper single crystals after initial construction are relaxed by conjugate gradient method and then equilibrated at 300 K using NVT ensemble for 100 ps with a time step of 0.002 ps under periodic boundary conditions. Temperature is held constant using Nose-Hoover thermostat[16], [17]. The equilibrated samples are then subjected to irradiation by PKA[4], [18] method in which only one initial chosen Cu atom is given PKA velocity (Figure 1c) along the three directions (x, y and z) corresponding to 0.5keV, 1keV, 2keV, 3keV, 4keV and 5keV energies. The velocity vector corresponding to the above energies is [2 1 1]. We used a 4Å thick thermostat layer on all sides to simulate bulk temperature of 300 K. The damage region is ~ 40 Å along height and thickness as observed from the studies of Averback et al. [19] on copper single crystal by PKA method. So the present simulation domain is well enough to study the irradiation damage. Irradiation is carried out in three stages of time-steps (0.01fs, 0.1fs and 1fs) with a total time of 5 ps to maintain the system in equilibrium with increasing temperatures under NVE ensemble and periodic boundary conditions. After irradiation process, the samples from the final stage of radiation (radiation time = 5 ps) are extracted and equilibrated at a temperature of 300 K under periodic boundary conditions using NVT ensemble for 50 ps. After relaxation, the samples are subjected to uniaxial tensile deformation. The sample is divided into rigid regions (15 Å each) and mobile region (Figure 1d) to simulate a uniaxial tensile loading. The tensile test is conducted by pulling the top rigid region at a uniform velocity corresponding to strain rate of $10^{10}$ s$^{-1}$. The temperature is held constant at 300 K by using Nose-Hoover thermostat and non-periodic boundary conditions is applied. Similar boundary conditions are applied in the studies of Spearot et al. [20] and Wan et al. [10]. NVT ensemble and timestep of 0.002 ps is used in the tensile simulation. The atomic level stress is calculated using virial stress[21]. We used OVITO simulation software [22] to observe crystal defects such as vacancies, deformation mechanism features such as dislocations in the irradiated and deformed copper single crystals.

3. Results and Discussions

3.1 Stress-strain response of un-irradiated copper single crystal

Figure 2a depicts the stress-strain response of un-irradiated copper single crystals of [100] and [110] orientations. The snapshots of defects, such as stacking faults (Figures 2a, 2c) and dislocations (Figures 2b, 2d) evolved during deformation are also captured at strains where significant changes occur in the stress-strain curve. As seen from Figure 2a, both the stress-strain curves show elastic–plastic stress-strain behavior. For the sample with [100] orientation, stress is proportional to strain up to strain of $e = 0.05$ reaching a maximum stress of 2.2 GPa. Defect analysis reveals that there are no dislocations observed up to this strain. The slope of the stress-strain curve in this region gives the modulus of elasticity, $E$ which is equal to 53.85GPa ($E = 61.89$ [5]). Straining beyond this point, the copper single crystal undergoes plastic deformation by dislocation slip on {111} plane resulting in a sharp drop in the stress. Similar flow softening behavior is reported in the Cu grain boundary deformation studies carried out by Spearot et al [20]. The drop in the stress is evident from the dislocations emitted at strain $e = 0.08$. At this strain, we observe Shockley partials (green colour) and stair rod (pink colour) dislocations. The Burgers vector, the type of few dislocations at the above strain are $1/6 [-2 -1 -1]$ (screw); $1/6 [1 -1 0]$ (edge) and $1/6 [2 -1 1]$ (mixed) and are shown in the zoomed regions (Figure 2b). It is well known that Shockley partial
dislocations are formed due to dissociation of perfect dislocation[23], and stair rod dislocations are formed by the reaction between the partials[24]. Further, Shockley partials contain stacking faults[25]. In the present study, we also observed stacking faults, which are captured by removing perfect fcc and surface atoms. Gao et al. [26] also reported Shockley partial dislocations in the deformed copper single crystals using MD simulations. In the present study, beyond the strain of $e = 0.1$, the sample continues to deform plastically. The corresponding snapshots of defects reveal higher defect density comprising of stacking faults and dislocations. It can be noted that there is the absence of periodic stepwise relaxation behavior (saw-tooth shaped stress-strain curve which is commonly observed at the nanoscale) indicative of higher disorder in the crystal lattice under high strain rate conditions[27]. Also, it can be due to the nucleation of multiple slip systems at the same time and thus frequent dislocation interactions leading to smaller fluctuations of flow stress[28].

**Figure 2.** Stress-strain curves of un-irradiated copper single crystals of [100] and [110] orientations. Atomic snapshots with (a, c) Stacking faults; (b, d) Dislocations captured at different strains.

The stress-strain behavior of the [110] oriented copper single crystal also shows elastic-plastic behavior similar to [100]. The stress reaches a maximum of 1.5GPa ($e = 0.03$), thereafter, the sudden drop occurs due to yield. The corresponding defect analysis reveals several Shockley partial dislocations which are an indication of dislocation-mediated plasticity. The Burgers vector and type of dislocation of a Shockley partial at the above strain is identified to be $1/6 [1 -1 -2]$(mixed) and is shown in the zoomed region (Figure 2d). Due to the interactions between the dislocations, the dislocation density increases and also the formation of stair rod and some unknown dislocations (red colour; $e = 0.04$). The calculated Young’s modulus from the slope of the initial linear portion of the stress-strain curve is 62.7 GPa which is higher as compared to the [100] orientation. The stress is found to be more serrated and could be due to the activation of fewer slip systems after yielding and leading to dislocation starved condition [28].

### 3.2 Defects in copper single crystals due to irradiation

Figure 3A shows the plot of total number of vacancies generated due to irradiation at different energies in the copper single crystals of different orientations. The numbers of defects are analyzed with Wigner–Seitz cell method [5] which is implemented in OVITO[22]. Also, the number of interstitials (not reported in the present study) almost have a linear relation with the number of vacancies. From the plot, it can be
seen that number of vacancies increase with irradiation energies up to 2 keV, followed by a drop and again rise in the number of the vacancies. Li et al. [5] also reported such fluctuations in the number of vacancies with increasing incident energies. In the above study, 189 vacancies are reported at an irradiation energy of 5 keV, whereas 150-225 vacancies are observed in the present study. The difference could be due to irradiation technique and also the size of the sample. Further, due to electronic stopping at higher irradiation energies (3 keV-5 keV) the vacancies are found to be decreasing. Figure 3B shows the atomic snapshots of the irradiated copper single crystal with different orientations containing vacancies and Shockley partial dislocations generated at irradiation energies at 0.5 keV and 1 keV. It is reported that Shockley partials are observed due to dislocation interaction with the defects (vacancies, interstitials) [29], [30]. Figure 3C shows the projection of atomic configurations in 25 Å thick slab of [100] oriented copper single crystal irradiated at 4 keV irradiation energy. From the figure, the regions where crystallinity is destroyed can be clearly observed. Liquid like regions are observed in the sample after an irradiation time of 5 ps. Bacon and Rubia [31] also found disorder, liquid like zones in the irradiated Cu. In summary [110] oriented copper single crystal is less prone to radiation damage with an increase in irradiation energy.

Figure 3A) Number of vacancies generated at different irradiation energies in copper single crystals of [100] and [110] orientations. B) Atomic snapshots showing the formation of vacancies and Shockley partial dislocations in the irradiated samples at 0.5 keV and 1 keV irradiation energies. C) Projection of atomic configurations in 25 Å thick slab of [100] oriented copper single crystal irradiated at 4 keV irradiation energy.

Structural changes from the center of the PKA to a distance of 5 Å and 10 Å radius are studied using RDF (radial distribution function) analysis for both the orientations. Figure 4A shows the RDF plots of the 10 Å diameter regions for two different orientations at an irradiation energy of 4 keV. As seen from Figure 4Aa for [100] orientation, the initial structure is crystalline with sharp, intense peaks, but with the progress of irradiation (0-5 ps) crystalline order is destroyed and amorphization is induced which is seen in the form of small and diffuse peaks and disappearance of peaks at 5Å, 6Å and 7Å radius. Similarly, in the copper single crystal with [110] orientation (Figure 4Ab), crystallinity is destroyed with irradiation time (0-5 ps), but to a greater extent as observed from the lower intense, and broad first peak. Also, there is no splitting of the first peak as observed in [100] oriented sample at 5ps which indicates amorphous nature. Figures 4Ba and 4Bb show the RDF plots for the 20 Å diameter region of [100] and [110] orientation. As
compared to the 10 Å diameter regions the crystallinity in these regions is not lost to a greater extent in both the oriented copper single crystals.

Figure 4. RDF plots of 5 Å radius (A) and 10 Å radius (B) regions from the center of PKA of [100] and [110] oriented copper single crystals.

During irradiation, atomic mixing occurs due to the relocation of atoms and is important for predicting the phase stability and synthesis of new materials [18]. To investigate the atomic mixing, MSD (mean square displacement) [18], [32] calculations are carried out for the irradiated samples. Figures 5a and 5b show the MSD vs. time plots of [100] and [110] oriented samples at different irradiation energies in the range of 1keV-5keV. MSD curves show two regions (ballistic and diffusive) which are typically observed for any irradiated material. Similar features are also observed in the MD simulation displacement cascades studies of Cu at 5 keV irradiation energy, and an MSD value of $5.1 \times 10^4$ Å$^2$ is reported [18]. In the present study, we find that the value of total mixing in [100] orientation is the highest at 4 keV irradiation energy and is $4.4 \times 10^4$ Å$^2$. For the copper single crystal with [110] orientation (Figure 5b), the total MSD at 5 keV is $8.9 \times 10^4$ Å$^2$ which is much higher than that observed in [100] orientation, indicating higher atomic mixing in this orientation. Table 1 shows the self-diffusivity values of copper for both the directions and at different irradiation energies that are calculated from the slopes of the diffusive region in the radiation time range of 3-5 ps. It is observed that in the copper single crystal with [110] orientation, the atomic mixing is more as compared to the other orientation except for irradiation energies of 1keV and 2keV.
Figure 5. MSD vs. timestep plots of the copper single crystals calculated at a distance of 10 Å radius from the center of PKA for different orientations: a) [100]; b) [110].

Table 1. Self-diffusivity values of copper at different irradiation energies in both the crystallographic directions. Approximate value of self-diffusivity of Cu obtained from literature is shown in parenthesis.

| Incident energy (keV) | [100] (m²/sec) | [110] (m²/sec) |
|-----------------------|----------------|-----------------|
| 1                     | $4.68 \times 10^{-5}$ | $4.05 \times 10^{-5}$ |
| 2                     | $10.43 \times 10^{-5}$ | $8.28 \times 10^{-5}$ |
| 3                     | $6.50 \times 10^{-5}$ | $17.43 \times 10^{-5}$ |
| 4                     | $12.53 \times 10^{-5}$ | $25.21 \times 10^{-5}$ |
| 5                     | $9.37 \times 10^{-5}$ | $27.36 \times 10^{-5}$, $(8 \times 10^{-4})$ [18] |

3.3 Stress-strain response and mechanical properties of irradiated copper single crystals

Figure 6. Stress-strain response of irradiated Cu single crystals at different irradiation energies for different orientations: a) [100]; b) [110]. For clarity, the peak stress regions are zoomed and shown in the inset.
After irradiation, the copper single crystals are subjected to uniaxial tensile deformation along the axial direction at a temperature of 300 K and strain rate of $10^{-10}$ s$^{-1}$. Figures 6a and 6b show the stress-strain response of the irradiated samples of [100] and [110] orientations at different irradiation energies in the range of 0.5keV-5keV. It can be observed that the peak stresses of all the irradiated Cusingle crystal samples are lower than the un-irradiated Cu samples and overall decreases with increase in irradiation energies. However, there are few exceptions at irradiation energies of 3 and 4 keV in [100] orientation and 2, 3 and 5 keV in [110] orientation. The smaller value of peak stress of irradiated samples as compared to the un-irradiated samples is attributed to the atomic relaxation in the presence of defects (vacancies).

Figure 7. Variation of Young’s modulus with irradiation energy (a) and number of vacancies (b) for the copper single crystals of [100] and [110] orientations.

Figure 8. Variation of yield strength with irradiation energy (a) and number of vacancies (b) for the copper single crystals of [100] and [110] orientations.

A comparison of Young’s modulus values against irradiation energies and number of vacancies are shown in Figure 7a and Figure 7b for the copper single crystals of [100] and [110] orientations. The zero incident energy denotes the case of the un-irradiated sample. It is observed that Young’s modulus decreases dramatically when the irradiation energy is less than 1 keV in [110] orientation. On the other hand, the decrease in modulus is very less for the sample with [100] orientation. At higher irradiation energies, it is found that there is no obvious relation between Young’s modulus and irradiation energy in both the samples. To analyze further, we plot Young’s modulus versus number of vacancies for different irradiation energies as shown in Figure 7b. Due to the presence of vacancies in the irradiated samples, Young’s modulus decreases and the decrease is proportional to the number of vacancies for both the orientations. Figure 8a and Figure 8b shows the plot of yield strength variation with irradiation energy and
number of vacancies for the copper single crystals of two different orientations. It is found that, under tensile loading, yield strength decreases with the increase in irradiation energies and number of vacancies. The decrease is more in the copper single crystal with [100] orientation. This implies that yield strength along the particular crystallographic direction is contributed by the vacancy mechanism.

3.3.1 Dislocation analysis

Figure 9. Snapshots of dislocations generated at strains $e = 0$ to $e = 0.1$ at different irradiation energies in the copper single crystals of [100] (a) and [110] (b) orientations. Burgers vector and type of dislocations in A and B regions are indicated in the zoomed regions.

Dislocation analysis is vital to understand the underlying deformation mechanism. Figures 9a and 9b shows the snapshots of dislocations evolved during deformation of the irradiated samples at strains $e = 0$ to $e = 0.1$ for [100] and [110] orientations. It is clear from the images that copper single crystals are free from dislocations in the elastic region under un-irradiated condition. Due to irradiation, defects such as vacancies and Shockley partial dislocations are observed in the undeformed copper single crystals, i.e., at strain $e = 0$. As the samples are strained to the elastic limit, the interactions between vacancies and dislocations result in an increase in Shockley partial dislocation density which is clearly seen at strains $e = 0.03$ ([100]) and $e = 0.02$ ([110]). However, there are few exceptions at irradiation energies of 0.5 keV in [100] oriented sample and 5 keV in [110] oriented sample. Also, few perfect dislocations (blue color) are
observed in the samples at strain $e = 0.03$ (5 keV) in [100] and at strain $e = 0.02$ (4 keV) in [110] orientations. After the yield strain, there is a sudden burst of dislocations in both the samples ($e=0.07$ and $e = 0.04$). Upon straining further ($e = 0.1$), a decrease in Shockley partial dislocation density is observed. Burgers vector and type of dislocation of few dislocations evolved at strains $e = 0.07$ ([100]) and $e = 0.04$ ([110]) at 1 keV irradiation energy are shown in the zoomed regions ‘A’ and ‘B’. Thus, it can be concluded that the deformation mechanism in the Cusample is mainly by Shockley partial dislocation.

3.3.2 Dislocation density
Calculation of dislocation density in un-irradiated and irradiated copper single crystal is necessary to further quantify the role of crystallographic orientation and irradiation on plastic deformation. In the un-irradiated samples, the dislocation density is found to be maximum after the yield due to sudden burst of dislocations ($6 \times 10^{16}$ m$^{-2}$ at $e = 0.07$ for [100] and $34 \times 10^{16}$ m$^{-2}$ at $e = 0.04$ for [110] orientations). Thereafter, dislocation density decreases with strain due to the annihilation of dislocations[33]. Sichani and Spearot[34] reported that orientation has a significant effect on the evolution of dislocation density during shock loading of copper ($\sim 2 \times 10^{17}$ m$^{-2}$ is observed at 20 GPa pressure in <110> orientation and time = 20 ps). In the present study, due to irradiation, there is certain amount of dislocation density (at strain $e = 0$), and is $\sim 1 \times 10^{16}$ m$^{-2}$ in [100] orientation, whereas in [110] it is $0.8 \times 10^{16}$ m$^{-2}$. As the copper single crystals are strained to the elastic limit ($e = 0.03$; $e = 0.02$) the dislocation density increases. The increase is more prominent in the sample with [100] orientation at 2 keV and 5 keV irradiation energies than [110] oriented sample. Beyond the yield, the dislocation density increases abruptly at all the irradiation energies, and the magnitude of dislocation density is much higher in the sample with [110] orientation which is in the range of $17 \times 10^{16}$ m$^{-2}$ - $30 \times 10^{16}$ m$^{-2}$.

4. Conclusions
Based on the MD simulations carried out, we found that the extent of radiation damage and the mechanical properties of [100] and [110] oriented copper single crystals are found to be different. It can be concluded that the vacancies and Shockley partial dislocations are induced due to irradiation, and [110] oriented sample is less prone to radiation damage with an increase in irradiation energy. The structural studies indicate that crystallinity is destroyed at 5 Å radius from the center of PKA in both the orientations, but to a greater extent in the [110] orientation. The extent of atomic mixing is found to be higher for [110] orientation at 5 keV radiation energy. Finally, irradiation deteriorates stiffness and yield strength of the copper single crystals. The results are important in the prediction and performance of the materials applications in nuclear reactors.

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