Deformation of Ni\textsubscript{20}W\textsubscript{20}Cu\textsubscript{20}Fe\textsubscript{20}Mo\textsubscript{20} high entropy alloy for tensile followed by compressive and compressive followed by tensile loading: A molecular dynamics simulation based study

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Abstract. In this paper, molecular dynamics (MD) simulations based study on deformation behavior during uniaxial tension followed by compression and compression followed by tension after 0.6 pre-strain for Ni20W20Cu20Fe20Mo20 high entropy alloy (20 at. % each element) single crystals has been reported. This MD simulation is carried out at strain rate of 10\textsuperscript{8} s\textsuperscript{-1} and at the temperature of -10\textdegree C. The influence of observed nano twin on deformation behaviour for such two types of loading process (i.e. tensile followed by compressive and compressive followed by tensile) has been investigated thoroughly. It is found that the dominant deformation mechanism is twin for tensile forward loading in Ni20W20Cu20Fe20Mo20 high entropy alloy single crystal, whereas atomic diffusion is the dominating factor for deformation behaviour in compressive reverse loading direction of high entropy alloy.

Keywords: Molecular Dynamics; High entropy alloy; Twin; Atomic diffusion

1. Introduction
An equi-molar solid solution of five or more principal metallic elements having high entropy of mixing is known as High-entropy alloys (HEA) [1]. These kind of multi-component alloys are usually comprised of metallic element with a concentration between 5 and 35 at. % each. According to experimental findings reported in literature, higher mixing entropy of these alloys leads to the formation of solid solution phase having similar structure and consequently restricts formation of different phases [1]. HEAs have some advantageous properties like high strength/hardness, outstanding wear resistance, exceptional high-temperature strength, good structural stability, good corrosion and oxidation resistance. Moreover, these alloys are highly irradiation resistant. During particle irradiation, the high atomic-level stress facilitates amorphorization followed by local melting and re-crystallization. This process leaves fewer defects in HEAs as compared to conventional alloys which makes HEAs applicable for high temperature applications like nuclear sectors [2]. HEAs can also be used as a coating material for anti-sticky molds, and material having diffusion barrier application because they have amorphous structure and low roughness. HEA has also potential application as brazing filler, for welding cemented carbide and steel [3]. The HEAs have better fatigue properties in comparison with conventional alloys, such as steels, titanium alloys, and even advanced bulk metallic glasses [4]. The recent discovery and development of high-entropy alloys has opened the door to introduce customization in stacking fault energy of materials which in turn to help to design material having high mechanical strength. High-entropy alloys (HEAs) can have either high strength or high ductility, but achievement of both at same time is still facing a serious challenge [1]. The inferior cast ability and compositional segregation of HEAs also limit their
technological applications. To tackle these problems, here we have proposed a novel strategy to design HEAs using molecular dynamics simulation. Experimental studies on the deformation mechanism is difficult as it has numerous drawbacks such as gripping of the samples, rotation of the samples, expensive setups to maintain the high precision equipment/facilities and uncertainty in nano-scale measurements [5-8]. Classical molecular dynamics simulations (MD) have been emerged as an effective simulation method for studying the behaviour and underlying mechanism of deformation at atomic level [9-11]. According to simulation findings reported in literature, micro-structures and stress on the atomic level are important to appreciate the mechanical behaviors and relevant mechanisms by molecular dynamics [12]. According to author knowledge, tensile followed by compressive and compressive followed by tensile of HEAs are not still reported. A nano scale simulation using MD has been performed here to study deformation behavior of HEA (Ni_{20}W_{20}Cu_{20}Fe_{20}Mo_{20} high entropy alloy (20 at. % each element)) at low temperature during tension followed by compression and compression followed by tension loading. In addition, twinning and amorphization along with their features and interactions are also investigated.

2. Computational details

Classical MD simulation deformation studies of high entropy single crystals alloy have been performed using Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS, Sandia National Laboratory, USA) [13]. Atomic positions and visualization of snapshots are done using open visualization tool software OVITO [14, 15]. In the present study we used EAM (embedded atom method) potential developed by Zhou et al. [16] to model the interactions between Ni, W, Fe, Cu, and Mo atoms. The expression for total energy of the crystal is given below

$$E = \frac{1}{2} \sum_{i,j,|i-j|} \phi_{ij}(r_{ij}) + \sum_i F_i(\rho_i)$$

where $\phi_{ij}$ represents the pair energy between atoms $i$ and $j$ separated by a distance $r_{ij}$, and $F_i$ is the embedding energy associated with embedding an atom $i$ into a local site with an electron density $\rho_i$.

In the present study single crystal Ni sample is prepared by creating a perfect FCC crystal of Ni with lattice constant of 3.52 Å and Ni-W-Fe-Cu-Mo alloys are created by randomly replacing Ni atoms of the single crystal by W, Fe, Cu, Mo atoms (20 at. % each). The samples are cylindrical in shape with 100 Å diameter and 100Å in length as shown in Fig. 1 and comprises ~72300 atoms. After the initial atomic configuration, the samples are relaxed by the conjugate gradient algorithm through local energy minimum for 100 ps at temperature of -10 °C. The samples are subjected to uniaxial tensile-compressive and compressive-tensile loading separately along Y-direction [010] under periodic boundary condition along loading direction simulated at -10 °C and at strain rate of 108 s^{-1}. Simulations are performed under NVT ensemble, integrated by velocity-Verlet algorithm with a time-step of 0.002 ps.
3. Results and discussion

3.1. Stress-strain behaviour

The stress-strain curves for high entropy alloy single crystal under uniaxial loading (tension and compression) simulated at -10 °C temperature and strain rate of 108 s⁻¹, are shown in Fig. 2. Four different stages, i.e. a linear elastic region, a small plastic region, and again a linear elastic region followed by plastic deformation are observed in both tensile and compressive stress-strain curves for high entropy alloy single crystal.

Fig.1: Atomic configuration 3-D snapshots of HEA sample (a) initial structure and (b) CSP of initial structure

Fig.2: Engineering stress-strain curves for high entropy alloy single crystal under uniaxial loading.
The tensile stress of maximum value is ~1.9 GPa corresponding to strain ~0.25. On other hand, the compressive stress of maximum value is ~4.4 GPa corresponding to strain ~0.19. The small plastic portion of the tensile and compressive curve are due to twin formation. After small plastic deformation followed by linear elastic portion of the tensile and compressive curve are due to strain hardening. The stress-strain curves of high entropy alloy single crystals for tensile followed by compressive loading after ~0.60 pre strain and the pictorial representation of corresponding atomic snapshots colored according to CSP (Centro symmetric parameter) values at different position of deformation path have been presented in Fig. 3.

It is revealed from Fig. 3 that the presence of plastic deformation feature is presented of forward loading direction and twin are observed at a1 point of stress-strain curve during tensile part of the loading. On the other hand, crystalline and amorphous structure are observed during compressive part of the loading reversed after 0.6 strain. The stress-strain curves of high entropy alloy single crystals for compressive followed by tensile loading after ~0.60 pre strain and The pictorial representation of corresponding atomic snapshots colored according to CSP values at different position of deformation path have been presented in Fig. 4. It is revealed from Fig. 4 that the presence of plastic deformation feature is presented of forward loading direction and twin are observed at a1 point of stress-strain curve during tensile part of the loading. On the other hand, crystalline and amorphous structure is observed during compressive part of the loading reversed after 0.6 strain. Linear elastic region and serrated plastic region are observed. Further, reverse loading at different direction after which yield stress more in compressive followed by tensile type of loading with respect to tensile followed by compressive type of loading of high entropy alloy. The generation of twins are observed mostly during forward loading (i.e. tensile part of tensile followed by compressive and compressive part of compressive followed by tensile) and subsequently these twins are found to act as potential sources of amorphous formation. This phenomenon is not reported in available literature for single crystal during tensile followed compressive type of loading.

Fig.3: Engineering stress-strain curves of high entropy alloy single crystals for tensile followed by compressive loading after ~0.60 pre strain with the atomic snapshots marked on corresponding point of stress-strain curve.
and compressive followed tensile type of loading. Twins are found to be inclined at $\sim 45^\circ$ to the loading direction.

Fig. 4: Engineering stress-strain curves of high entropy alloy single crystals for compressive followed by tensile loading after $\sim 0.60$ pre strain with the atomic snapshots marked on corresponding point of stress-strain curve.

3.2. Radial distribution function (RDF)

The RDF patterns at different loading direction such as tension followed by compression and compression followed by tension loading after 0.60 pre-strain for high entropy alloy single crystals have been presented in Fig. 5 (a) and 5 (b) respectively. Sharp peaks observed at different strains indicate that there is no amorphization of the high entropy alloy single crystal during the forward or reverse loading. The stress-strain curves of high entropy alloy single crystal exhibits linear elastic behavior and serrated plastic behavior. This is due to the transformation from crystalline to partial amorphous structure which is also evident in RDF plots provided in Fig. 5.

Fig. 5: The radial distribution functions at different strains during (a) tensile followed by compressive and (b) compressive followed by tensile loading after $\sim 0.60$ pre strain.
3.3. Stress Distribution
Von Mises’ stress contours plots representing development of stress at vertical cross section of all the specimens at different strain of forward and reverse loading have been shown in Fig. 6. The stress distributions at different strain are observed to be almost homogeneous throughout the specimen and slight localization of stress field near the surface is identified at the point of reverse loading. There is no significant polarization of stress field in high entropy alloy single crystals at different strain of forward and reverse loading as evident in Fig. 6.

![Stress Distribution Contours](image)

Fig.6: Stress distribution at different strain (a) 0.002 (tensile), 0.6 (tensile) and 0.6 (compressive) during tensile followed by compressive and (b) 0.002 (compressive), 0.6 (compressive) and 0.6 (tensile) during compressive followed by tensile loading of high entropy alloy single crystals,

4. Conclusions
Molecular dynamics simulations have been carried out for Ni20W20Cu20Fe20Mo20 high entropy alloy (20 at. % each element) single crystals with EAM potential for studying the underlying deformation mechanism during tension followed by compression and compression followed by tension. This MD simulation reveals that plastic deformation in Ni20W20Cu20Fe20Mo20 high entropy alloy (20 at. % each element) single crystals due to the twin and atomic diffusion. Formation of high entropy alloy single crystal causes reduction in crystallinity significantly and this leads to decrease in dependence of deformation process on dislocation controlled mechanisms. Twin dominated deformation mechanism prevails during forward
loading. Deformation of high entropy alloy during reverse loading is controlled by atomic diffusion. Stress distribution throughout the system almost homogenous.

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