Deformation behavior and fracture of Al-CuZr nano-laminates: A molecular dynamics simulation study

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Background

- Aluminum based MMCs with micron size dispersion of hard particles like Al_2O_3, SiC or intermetallic compounds show high specific strength, which makes them potential structural materials for the aerospace, naval and automotive applications [1-2].

- The major problem with the ceramic reinforcement materials are their low wettability which results in a porous interface, and thus deteriorates mechanical properties [3].

- Metallic glasses (MGs) possess high strength ~ 2 GPa, large elastic strain limit ~2%. and metallic in nature. So they are potential reinforcement materials in metal matrices [4].

- In the recent times, different types of MG particles (Fe-based, Cu-based, Zr-based and Al-based) have been used as reinforcements in Al alloy matrix [5-8]. These studies report that the metallic glass particles significantly improved the mechanical properties of the composite. The mechanical properties of the composites are listed in Table 1.

Table 1 Mechanical properties of Al-MG composites.

Matrix	Reinforcement (metallic glass)	Processing route	T_m (K)	T_x (K)	Compressive mechanical properties of matrix and composite	Reference/year
Al-10%Mg (A520) alloy	Cu_{54}-Zr_{36}-Ti_{10} nano-particles	Powder metallurgy	723-878	810	YS=190 MPa (matrix) YS= 580 MPa (Composite)	[6] (2010)
Pure Al	$Zr_{57}Ti_8Nb_{2.5}Cu_{13.9}$-$Ni_{11.1}Al_{7.5}$ glassy powder	Powder metallurgy	930	716	UTS = 155 MPa (Matrix) UTS= 250 MPa (composite)	[7] (2009)
Al-2024 alloy	$Fe_{73}Nb_5Ge_2$-$P_{10}C_6B_4$ glassy powder	Powder metallurgy	850-940	850	YS=250 MPa (Matrix) YS= 403 MPa (composite)	[9] (2014)

- Metallic glasses are brittle in nature due to disordered atomic structure. Therefore, there is no dislocation mediated plasticity as observed in metals, rather the deformation is localized into shear bands [10].

- The presence of a ductile/crystalline phase can hider the propagation of shear bands in metallic glasses and improves the ductility [11].

- Crystalline/amorphous (C/A) metallic nanolaminates have been increasingly studied due to their excellent mechanical behaviors [12]. In C/A laminates the ductility is mainly due to the crystalline layers and the suppression of shear bands occurs when the amorphous layers are sufficiently thin.

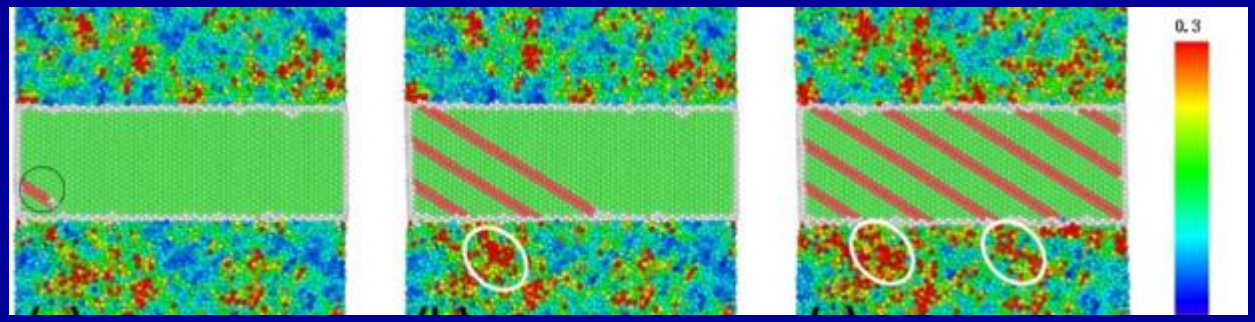

Fig. 1: Dislocations and STZ in Cu crystal and $Cu_{50}Zr_{50}$ metallic glass at different strains [12]

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GAPS in the literature

There are no studies reported on the Polycrstalline/Amorphous nanolaminates. The presence of polycrystalline could result in an increase in strength and plasticity of the laminates.

So in the present study we chose Al polycrystal and $Cu_{50}Zr_{50}$ metallic glass nanolimates as shown in Fig. 2

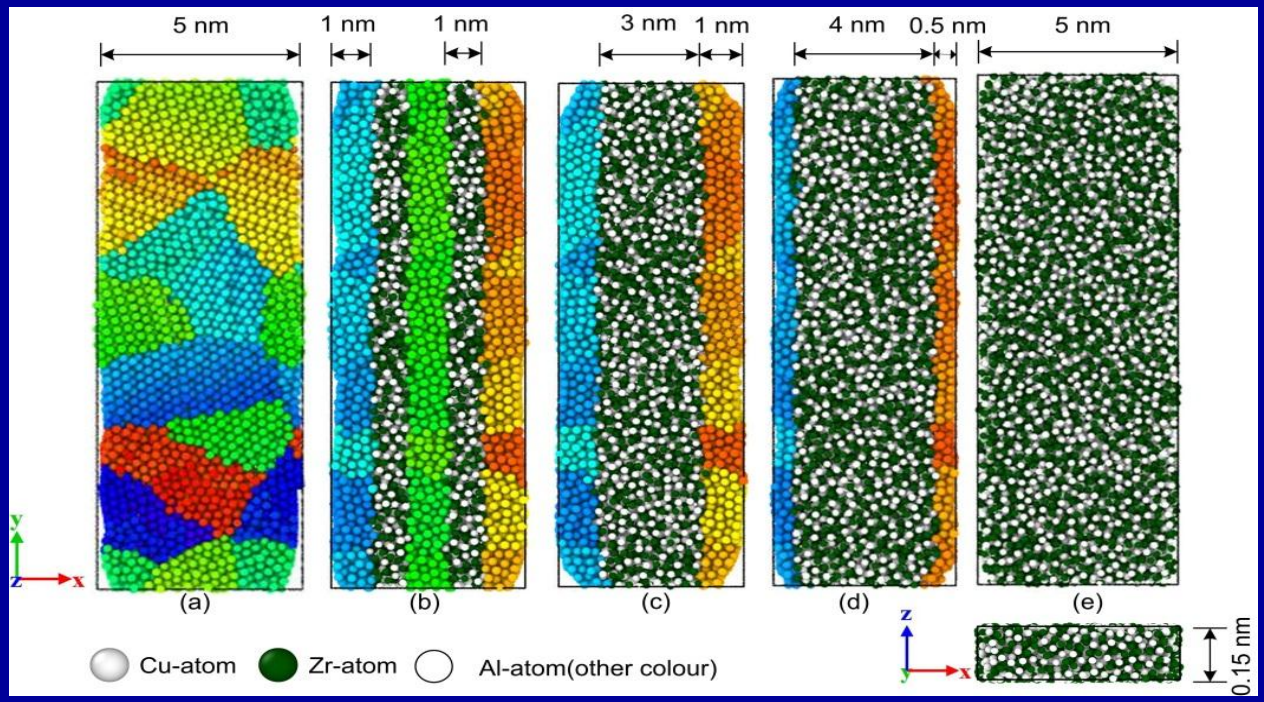

Fig. 2. Models with varying width of MG from 0 nm to 5 nm: (a) MG-0 nm (b) MG-1 nm (c) MG-3 nm (d) MG-4 nm (e) MG-5nm.

❑ Simulation methodology

- We performed atomistic simulations of deformation using molecular dynamics (MD) simulations.
- All the MD simulations are performed on LAMMPS platform [13].
- For defect analysis OVITO [14] software has been used.

❑ Sample preparation; interatomic potentials; boundary conditions and deformation method

- Al polycrystal and $Cu_{50}Zr_{50}$ metallic glass nanolimates with varying MG widths in the range of 0-5 nm are modelled and studied (Fig. 2).
- Nano-crystalline Al is generated with the help of open source command-line program Atomsk tool [15].
- $Cu_{50}Zr_{50}$ MG used in the construction of the models are generated by starting with an fcc copper supercell that is prepared by randomly generating the coordinates and replacing 50 % copper atoms by zirconium atoms [16].
- EAM potential developed by Zhou et al. [17] is used for modelling the interaction between the Al-Cu-Zr atoms during tensile deformation.

- NPT ensemble (where N = number of atoms; P = pressure; T = Temperature are fixed) is used in the simulations.

- To eliminate free surface effects and represent the realistic model, we have used periodic boundary condition on y-direction.

- The fracture strength of Al–$Cu_{50}Zr_{50}$ nano-laminate models is determined by applying tensile deformation along [010] direction (y-axis) parallel to the lamellae interface at strain rate of 10^{10} s^{-1} and temperature of 300 K.

- Temperature is held constant using Nose-Hoover thermostat.

- Strain is calculated by the ratio of change in the box length to the original length along y-axis and stress is calculated using Virial stress [18, 19].

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Results

Stress-strain behavior

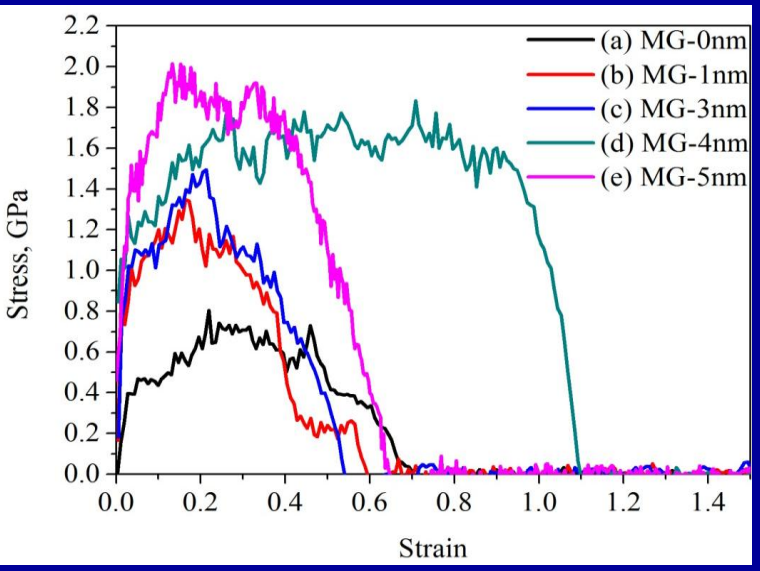
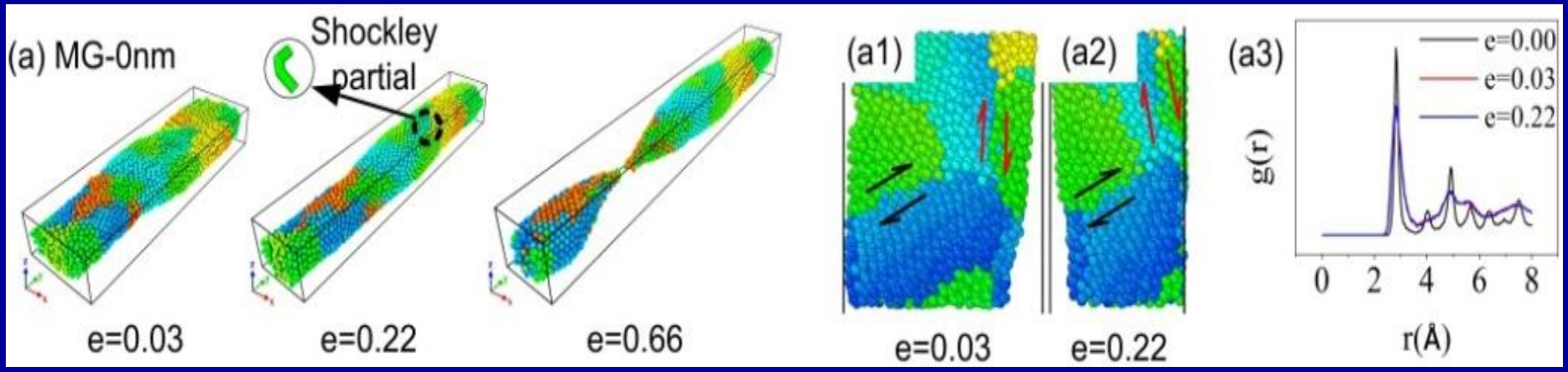


Fig. 3. Stress-strain plot of the Al-$Cu_{50}Zr_{50}$ interface lamellae models under mode-I loading with varying MG width from 0 nm to 5 nm: (a) crystalline Al of width 5 nm, (b) five alternate layers of nano-crystalline Al and MG ($Cu_{50}Zr_{50}$) each width of 1 nm, (c), two layers of nano-crystalline Al (1 nm each) and in between MG of width 3 nm, (d) two layers of crystalline Al (0.5 nm each) and in between MG of width 4 nm, (e) MG ($Cu_{50}Zr_{50}$) of width 5 nm.

- All the models show linear elastic region, strain hardening region followed by flow softening and finally fracture.
- The stress-strain curve for pure nano-crystalline Al model (Fig. 3a) of average grain size 2.5 nm begins with an elastic deformation from its initial state to the yield state σ_y (yield stress) = 0.4 GPa corresponding to strain of e = 0.03. At strain of e = 0.22 the stress reaches maximum, σ_{max}= 0.82 GPa. Straining of the Al model beyond e = 0.5 strain results in a sudden drop in the stress and finally fractures at strain of e=0.66.
- Fig 3b shows the stress-strain behavior of the laminate model having alternate layers of MG of 1nm width between nano-crystalline Al of 1 nm average grain size. The yield stress and peak stress are σ_y= 1.01 GPa and 1.36 GPa corresponding to the strains of e = 0.038 and e = 0.171. It is observed that in the presence of MG layers, the strength of the model is higher compared to the nano-crystalline Al model.
- Fig. 3c depicts the stress-strain response of the laminate model with 3 nm width MG placed in between the 1nm nano-crystalline Al. Similar stress-strain behavior is observed as in the model with 1 nm nano-crystalline Al. However, the strength is significantly higher ~ 1.5 GPa and is attributed to the presence of hard MG. Furthermore, in the model with 4nm MG (Fig. 3d) the strength is even higher. The stress-strain curve is flat beyond 0.4 strain and up to strain of e = 0.9
- The model with only MG (Fig. 2e) exhibits higher strength (2 GPa) as compared to the other models

Discussions

- Yamakov et al. [20] observed a yield strength of 2.3 GPa during deformation of nano-crystalline Al of grain size 45 nm.. Zhou et al. [21] studies have reported an inverse Hall-petch relation if the grain size decreases below 8 nm in nano-crystalline Cu and the plastic deformation occurs in the grain boundary, and by grain rotation. So, the lower yield strength of pure nano-crystalline Al in the present study is due to the inverse Hall-petch effect. CSP image shown below reveals the grain boundary sliding. Also amorphization occurs at large strains.



- As the MG layer is introduced into the nano-crystalline Al, and also with increasing its width, the deformation behavior of the laminate is found to be different from pure nano-crystalline Al and pure MG . This is attributed to the high strength of $Cu_{50}Zr_{50}$MG which bears the load upon loading.

References:
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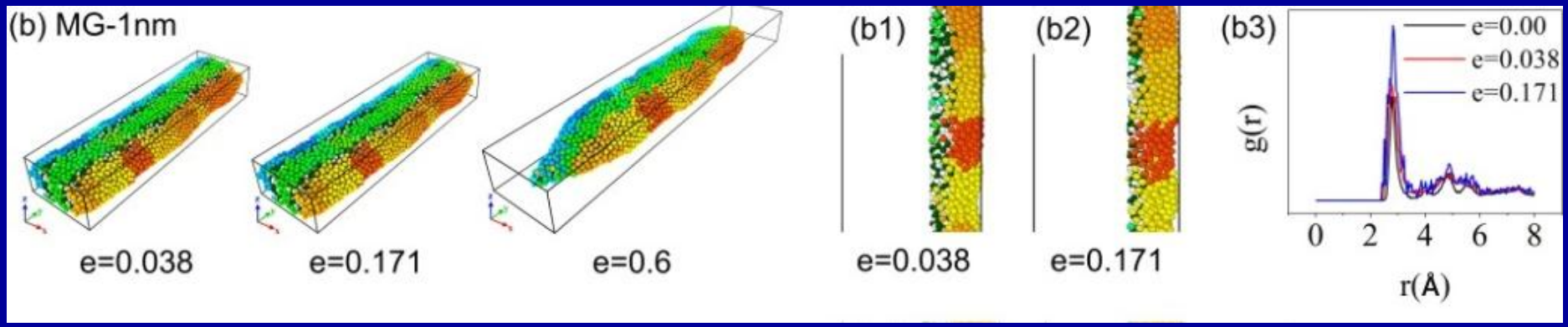
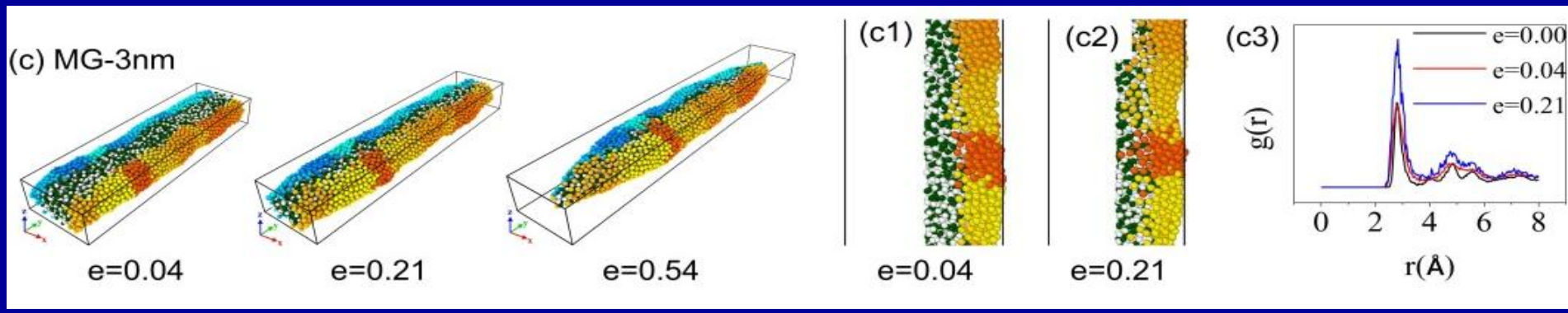
- Figure below shows the atomic snapshots of the laminate with 1 nm MG regions. At strain of e = 0.038 both the regions (Al and MG) are deformed plastically. With further straining due and to strong bonding at the interface between the MG and Al regions [22], grain boundary sliding and grain rotation is not significant as that observed in the pure nano-crystalline Al. Further, amorphization occurs at very less strain (e = 0.171) in the Al region as evident from the RDF plots. Also, no dislocations are observed during deformation and the model fractures at the ends at strain of e = 0.6



- With increase in MG width to 3 nm, the model elongates (e = 0.04 and e = 0.21) and fractures at strain of e = 0.54 which is less than 1 nm MG model. This is due to the presence of higher volume fraction of harder MG phase. The snapshots shows that there is no significant sliding or rotation of grain boundary, however there is amorphization of the Al region.



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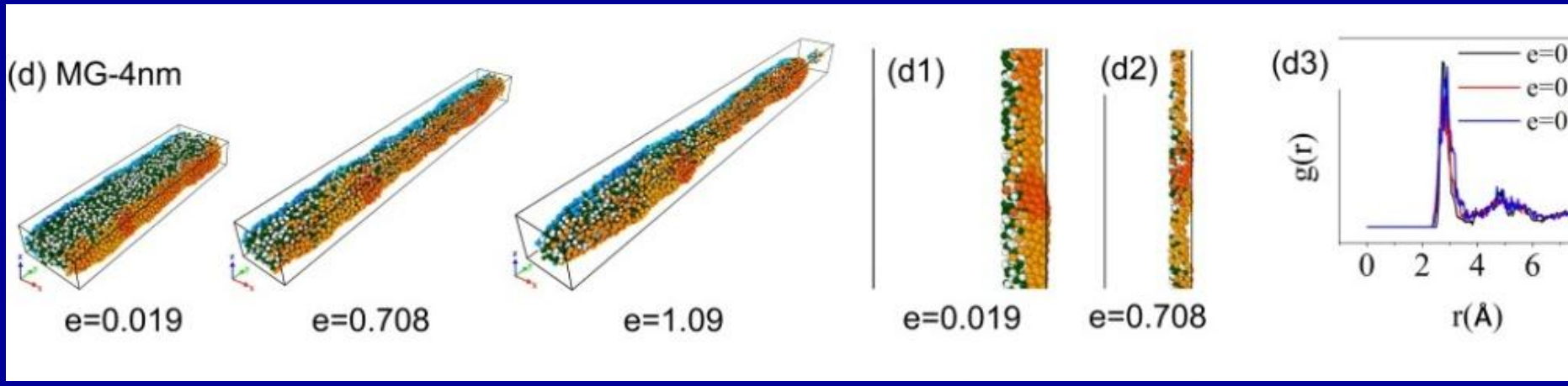
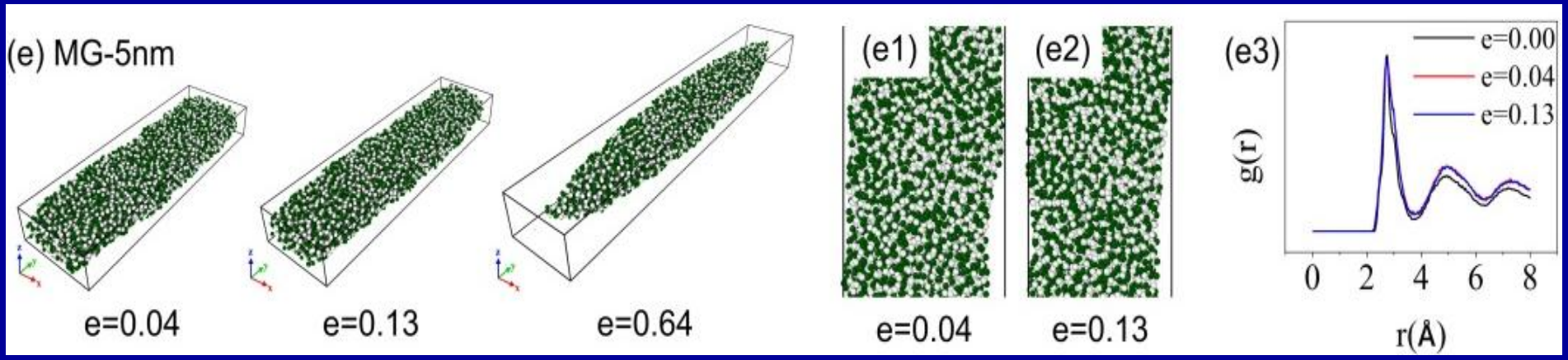
- In the model with 4 nm MG (Fig. 3d) the stress-strain curve is flat beyond 0.4 strain and up to strain of e = 0.9 which could be due to amorphization of Al region.



- In the case of pure MG model, uniform elongation occurs till strain of e = 0.13 and after which the model fractures in the ends of at strain of e = 0.64. The enlarged regions shows a decrease in cross-section and also neck like regions. The RDF plots shows low intense first peak and broad hump at different strains which is the characteristic nature of amorphous alloys.



Conclusions

We have performed molecular dynamics simulations to study the effect of different widths of $Cu_{50}Zr_{50}$ MG layers (1 nm-4 nm) in the Al-$Cu_{50}Zr_{50}$ (MG) nano-laminates. Based on the simulation results we draw the following conclusions.

- In the pure nano-crystalline Al, the plastic deformation is mainly dominated by grain boundary processes rather than dislocation mechanism. It is observed to be grain boundary sliding and grain rotation.

- Few Shockley partial dislocations are observed nucleating from the grain boundary. Also, amorphization of Al is observed at higher strains.

- With the introduction of MG layer, the strength of the laminate increases and is due the hard, disorder MG phase and also due to its different deformation mechanism. Also, no significant grain boundary sliding and rotation is observed in Al regions.

- We found that the laminate strength increases linearly with increase in MG widths at the loss of ductility. However, there is an exception in the case of model with 4nm MG width in which the strength and ductility is higher which needs to be further investigated.

- Finally, amorphization is observed in the Al regions in all the models at large strains containing MG and is due to the strong bonding at the interface regions and high strain rate of deformation.

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Thank you for your attention