Aluminum-$Cu_{64}Zr_{36}$ metallic glass interface study: Deformation behaviour, deformation mechanisms, structure, and fracture studies

Mentor : Dr. Pradeep gupta

Project members :

G.Kalpana reddy (19691a0360)

S.Mufiza anjum (19691a0362)

A.Balapothi reddy (19691a0315)

B. Abhilash (19691a0304)

Contents

- Introduction
- Literature review
- Gaps in literature
- Objective of research work
- Simulation procedure
- Boundary conditions

Introduction

Al-based metal matrix composites (MMCs) are of great interest owing to their remarkable mechanical properties, such as low density, high elastic modulus, strength and good wear resistance, which make them attractive for applications in the aerospace, automotive and defence .

The commonly used reinforcements are ceramic materials such as Al_2O_3 or SiC particles which possess an excellent combination of specific strength and stiffness at both ambient and elevated temperatures .

The major problem with the ceramic reinforcement materials are their low wettability which results in a porous interface, and thus deteriorates mechanical properties and increases corrosion sensitivity of the composite .

Metallic glass has better compatibility with the Al matrix and results in better interface bonding than conventional ceramic particles. In the recent times, different types of MGs particles (Fe-based, Cu-based, Zr-based and Al-based) have been used as reinforcements in Al alloy matrix .

Literature

Table 2.2. Mechanical properties of interface obtained under different modes of deformation (tensile and shear) by MD simulation studies

Model	Dimension (nm^3)	Potential	Boundary Conditions	Strain rate (s^{-1})	Yield strength (MPa)	Young modulus (GPa)	Maximum load (GPa)	Type of loading	Interface Model
Pure Al /SiC [12]	60×70×16	Morse potential	PSP	10^8s-1	180.6	224.42	4.23	Tensile	CZM
			PSP		156.3	188.66	3.52	Tensile*	
			SPP		76.6	180.63	3.05	Shear	
			SPP		66.45	177.93	2.56	Shear *	
Pure Al /Si [81]	25.6×14.78×1.145	MEAM potential	SPP	10^9s^{-1}	77.3	-	2.96	Tensile	interface
Al /α-Fe_2O_3 [82]	10×10×10	MEAM potential	PSP	10^8s^{-1}	80.1	-	-	Tensile	interface
Al /Al_2O_3 [83]	50×60×16	MEAM potential	PSP	10^8s^{-1}	-	201.88	4.24	Tensile	CZM
			PSP		-	186.77	4.18	Tensile*	
			SPP		-	78.6	3.2	Shear	
			SPP		-	71.43	3.12	Shear *	
Two brittle materials [84]	253×206×10 unit cell	Bulk interatomic potential	PSP	10^8s^{-1}	-	-	4.8	Tensile	CZM
					-	-	4.5	Shear	
A/ B [85]	80×65×3.2	AB Potential	PSP	10^8s^{-1}	-	-	4.3	Tensile	CZM
					-	-	2.2	Shear	
Cu/ Cu [18]	43.38×43.38×14.46 $Å^3$	EAM potential	PSP	10^8s^{-1}	-	-	14.4	Tensile	CZM
			SSP		-	-	2.6	Shear	
Al, Cu, Ni, Fe, Cr Single Crystal [16]	5×15×5 unit cell	Morse potentials	PSP	500 m/s	-	-	13.2	Tensile	Bilayer interface
					-	-	22.63		
					-	-	36.04		
					-	-	28.85		
					-	-	31.1		

Gaps in the literature

Metallic glass particles and flakes are used as reinforcements in Al metal matrix composites and it is reported that there is significant improvement in the mechanical properties of the composites as compared to the pure Al. The increase in the strength is attributed to the strong bonding at the interface as metallic glass is metallic in nature and good wettability. However, there are neither experimental nor simulation studies reported in literature on the interface characteristics between metal and metallic glass.

Defects, temperature play a vital role on the deformation behaviour and mechanism in metals. There are several literature studies that are reported on the crack propagation behaviour, influence of voids on the deformation behaviour in several interface models such as Al-SiC, Cu-SiC, bi-crystals. But, there are no atomistic or experimental studies related to the metal and metallic glass interface models.

Broad aims and objectives

To investigate Al (metal)-$Cu_{64}Zr_{36}$ (metallic glass) interface strength under mode-I (tensile) and mode-II (shear) loading conditions at temperature of 300 K

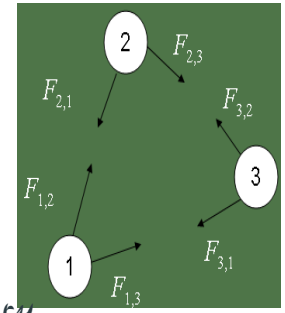
Simulation procedure

- How does an MD simulation run
- Boundary conditions
- Model Creation (still under simulation)
- Tensile simulation (in next phase)
- Shear simulation (in next phase)

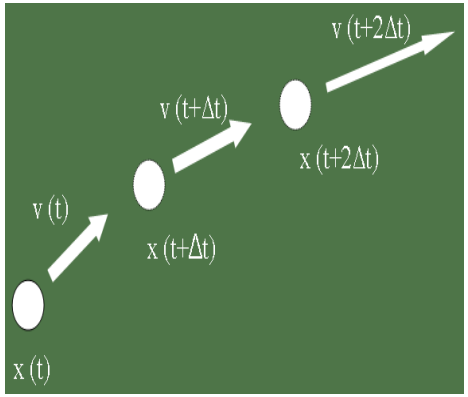
How does an MD simulation run ?

1. Initialize the positions and velocities of the atoms
2. Calculate forces/energy

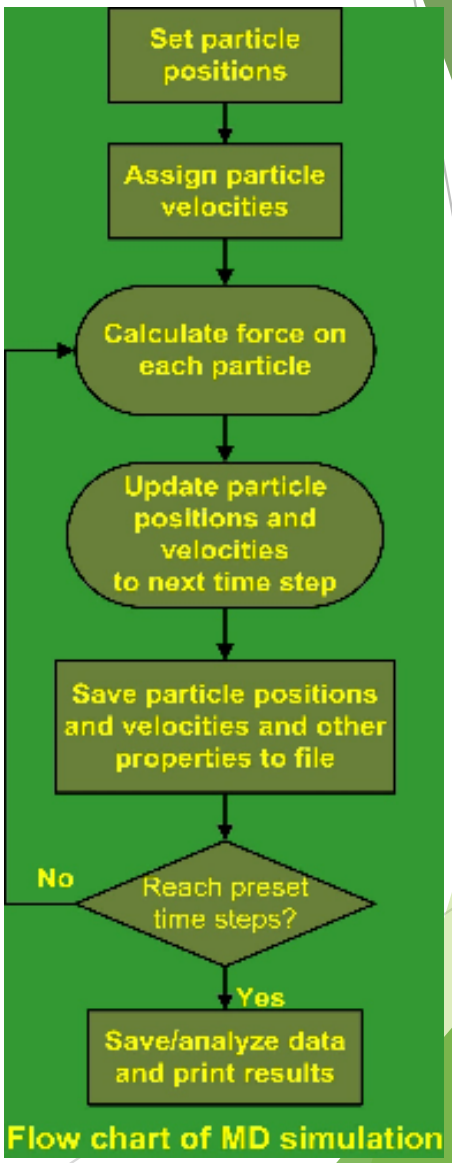
$$E_{total} = E_{bond} + E_{torsion} + E_{bond\text{-}angle} + E_{non\text{-}bond}$$



3. Calculate the forces on the atoms
4. Move the atoms and integrate Newton's equations of motion to obtain atomic trajectory

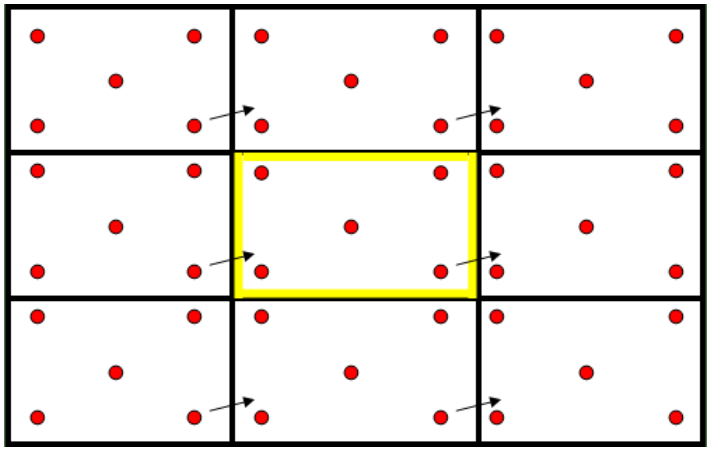


5. Update the new positions and velocities after time-step of 0.002 ps (Δt)



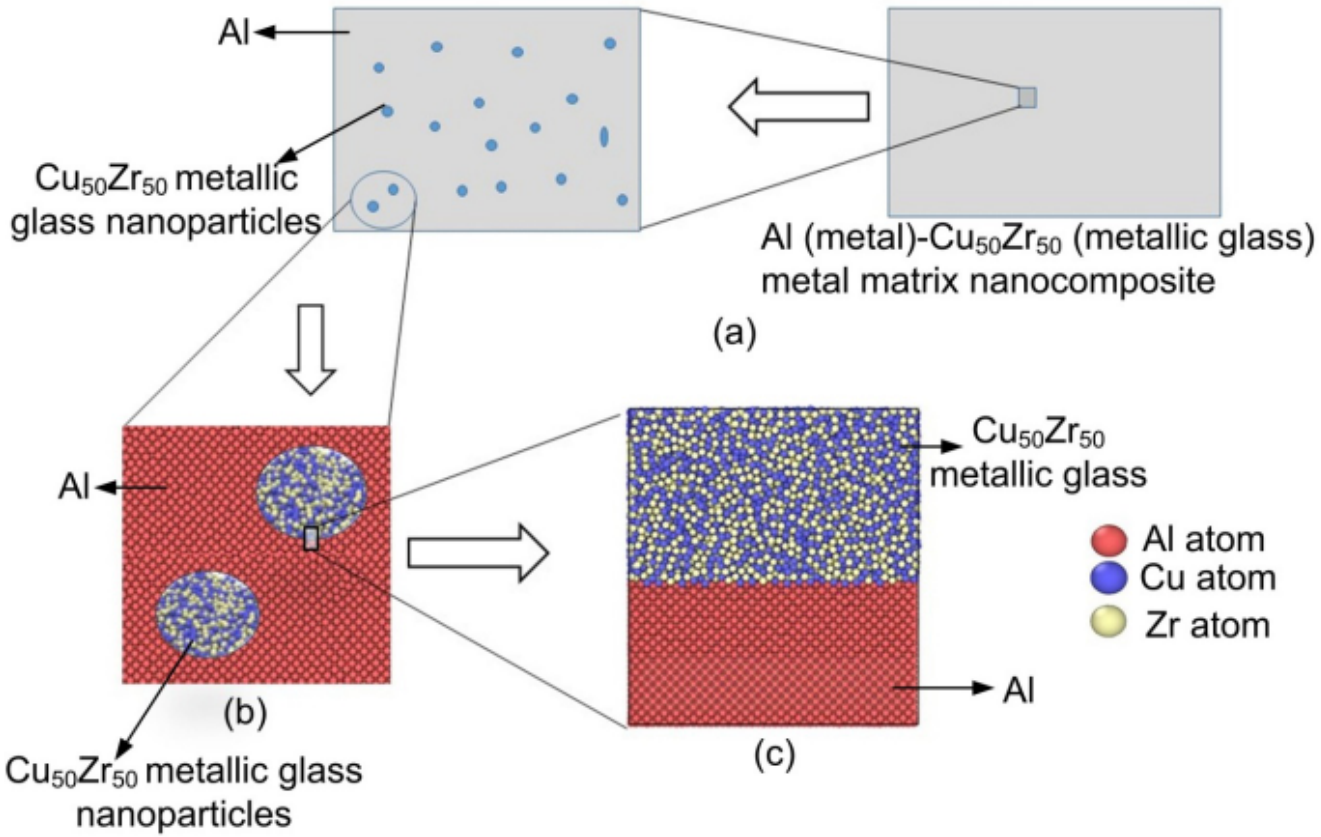
Boundary conditions

- Two major boundary conditions: isolated boundary condition (IBC) and periodic boundary conditions (PBC)
- IBC: particles interact among themselves but no interaction with outside
- PBC a super cell is considered in which atoms not only interact among themselves but also in the adjacent image supercells



An illustrative view of periodic boundary conditions

Model Creation



Thank You