EFFECT OF STRAIN RATE AND TEMPERATURE ON Al (METAL)-$Cu_{50}Zr_{50}$ (METALLIC GLASS) INTERFACE STRENGTH: A MOLECULAR DYNAMICS STUDY

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Introduction

Extensive use of metal matrix composite (MMC) in automobile, aerospace, civil structure and bio engineering applications has brought concern about the new technology for preparing, material characterization, properties, and production of these composites [1–4]. Metallic glasses (MGs) are fascinating as reinforcement because of its excellent properties such as higher elastic limit (~2%), high strength, good wettability and good corrosion resistance [5]. There are studies reported on the use of MG (Zr-based, Ni-based and copper based) as reinforcement in Al-matrix composites [6–8]. Interface plays a vital role in determining the strength of the composites. There are seldom studies reported on the interface characteristics. In the present study classical molecular dynamics (MD) simulations are performed to determine the Al-$Cu_{50}Zr_{50}$ interface strength chracteristics at strain rates of 10^9 s^{-1} and 10^{10} s^{-1} and at temperatures of 100 K and 300 K by subjecting the interface to mode-I loading.

Objectives and Methodology

Molecular dynamics (MD) simulations are performed to characterize the metal (Al)-metallic glass ($Cu_{50}Zr_{50}$) interface. Simulation box size of 100 Å (x) × 110 Å (y) × 50 Å (z) is used for the investigation the properties of model interface. The model is first constructed with the bottom layer (Al) of 50 Å and the top layer of 55 Å ($Cu_{50}Zr_{50}$) in height along y–direction. Thereafter, $Cu_{50}Zr_{50}$ metallic glass is obtained by rapid cooling at a cooling rate of 4×10^{12} K s^{-1} (fig.1) and for cracked sample void in introduced at the interface of diameter 10 Å. NPT ensemble is used in the above melt-quench studies.. EAM (Embedded Atom Method) potential is used for modelling the interaction between Al-Cu-Zr atoms. The fracture strength of Al–$Cu_{50}Zr_{50}$ model interface is determined by applying load in the directions normal to the interface.

Molecular dynamics (MD) simulations are performed using LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) [9]. EAM potential developed by Zhou et al. [2004] is used for modelling the interaction between the Al-Cu-Zr atoms during tensile deformation. As per the EAM, the total energy E of the crystal is expressed as below

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

where ϕ_{ij} represents the pair energy between atoms *i* and *j* separated by a distance *r* , and is the embedding energy associated with embedding an atom i into a local site with an electron density ρ_i .

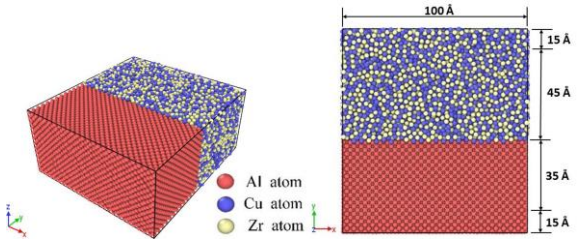

Fig. 1. Atomic snapshot of the sample with the help of OVITO [10]

Results and analysis

The stress strain results of the perfect interface (Fig. 2a and 2b) and cracked interface (Fig. 3a and 3b) deformed at strain rate of 10^9 s^{-1} and 10^{10} s^{-1} and simulated at temperature of 100K and 300 K respectively are presented here. Observed results are: 1. with the increase of strain rate results in increase stress, and 2. with the rise of temperature leads to the reduction of the stress, and 3. with the introduction of the crack in sample at the interface leads to reduction of stress as shown in (fig. 2). For the analysis of the dislocation and defects in the sample centrosymmetry parameter (CSP) snapshots are used (Fig. 3). Crack helps in fast nucleation of the defects such as slip and twins as shown in (Fig. 3(c-3)) due to which reduction in maximum stress is also observed. Due to low temperature and low strain rate strain hardening is also observed which leads to closer of the crack in (Fig. 3 (d-3)).

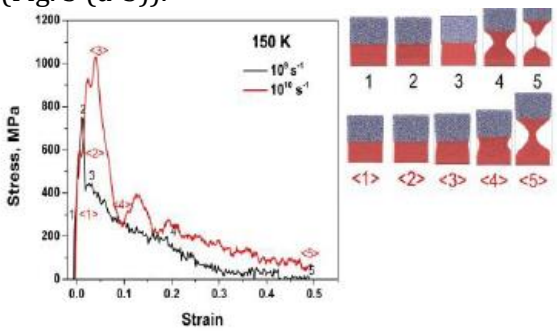

Fig.2. Stress-strain plot of the interface: (a) 100 K and (b) 300 K without crack and (c) at 100 K and (d) at 300 K with crack.

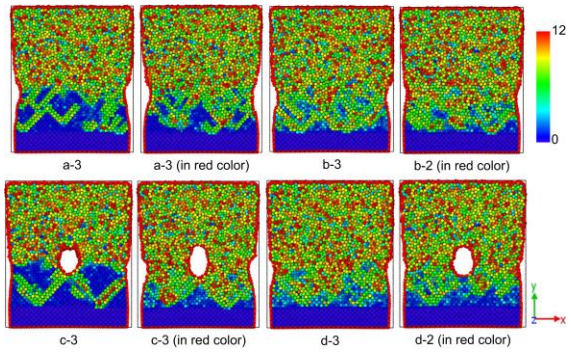

Fig. 3. Centrosymmetry parameter (CSP) snapshots of the samples corresponding to the stress-strain plots.

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