Mechanical Behaviour of Cu-Zr Binary Metallic Glasses: A Molecular Dynamic Simulation Study

N.H.Gamage, P.A.C.Madhushan, H.S.Sitinamaluwa*
Department of Material Science and Engineering, University of Moratuwa, Sri Lanka
**email: hansinees@uom.lk*

Metallic glasses (amorphous alloys) have gained increased attention in recent times due to their unique combination of mechanical properties such as high tensile strength, fatigue and wear resistance together with higher toughness values. However, the underlying deformation physics of these materials remain less firmly established as compared with crystalline alloys. One reason is the difficulty of characterization of material structure, as these materials do not have long range order in their atomic arrangements. Material modelling and simulation methods have paved new ways for the advancement of material development, modification and processing. For the study of amorphous materials, atomistic modelling and simulation techniques have proven to be very useful, as these techniques allow a closer look of local atomic environments of these materials.

In this research, molecular dynamics simulation is used to analyze mechanical behavior of Cu-Zr binary metallic glasses under tensile forces. Firstly, the relationship of toughness and strength over a range of atomic compositions of Cu-Zr metallic glasses (45 % Zr to 55 % Zr)is analyzed. In addition, the underlying deformation mechanisms of Cu-Zr metallic glasses were investigated. The MD simulations were done using Large-scale Atomic Molecular Massively Parallel Simulator (LAMMPS) and OVITO software is used for visualization and analysis of the simulation results.

As this study reveals, both fracture strength and toughness of Cu-Zr alloys are increased with increasing Zr content. Also, the Young's modulus of these alloys are also increased with the increasing Zr content. In-depth analysis of atomic structures suggests that the increasing free volume with increasing Zr content is responsible for high strength and toughness observed in the alloys with higher Zr content.

Keywords: Amorphous alloys, Bulk metallic glasses, MD simulation, Mechanical Properties