

Molecular Dynamics Studies on the Prediction of Interface Strength of Cu (metal)-CuZr (metallic glass) Metal Matrix Composites

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Abstract

The aim of this investigation is to predict the interface strength of metal (Cu-matrix)–metallic glass (Cu₅₀Zr₅₀-reinforcement) composites via molecular dynamics (MD) simulations. Simulation box size of 100 Å (x) × 110 Å (y) × 50 Å (z) is used for the investigation. At first Cu–Cu₅₀Zr₅₀ crystalline model is constructed with the bottom layer (Cu) of 50 Å and the top layer of 60 Å (Cu₅₀Zr₅₀) in height along y–direction. Thereafter, Cu₅₀Zr₅₀ metallic glass is obtained by rapid cooling at a cooling rate of $4 \times 10^{12} \text{ s}^{-1}$. The interface model is then equilibrated at 300 K for 500 ps to relieve the stresses. EAM (Embedded Atom Method) potential is used for modelling the interaction between Cu–Cu and Cu–Zr atoms. The fracture strength of Cu–Cu₅₀Zr₅₀ model interface is determined by tensile (mode–I) and shear (mode–II) loading. Periodic boundary conditions are applied along z–direction for shear while along x– and z–directions for tensile tests. A timestep of 0.002 ps is used for all the simulations. Tensile and shear tests are carried out at varying strain rates (10^8 s^{-1} , 10^9 s^{-1} and 10^{10} s^{-1}) and temperatures (100K and 300 K). The interface model is allowed for full separation under both the deformation modes. It is found that tensile as well as shear strength decrease with increase in temperature and increase with strain rate, as expected. Further, the maximum stress in shear is smaller than that in tensile at all strain rates and temperatures. Critical observations of the obtained results on Cu–Cu₅₀Zr₅₀ composites indicate better shear strengths as compared to the results of metal (matrix)-ceramic (reinforcement) composites available in the literature. Hence it can be concluded that metallic glass acts as a better reinforcement material than the popular ceramic reinforcements.

Key words: Molecular dynamics, tensile, shear, strain rate, temperature, interface.

1. Introduction

Composite is a blend of two materials, where one of the material is continuous called as matrix and which surrounds the second phase called as dispersed phase. There are several types of composites namely metal matrix composites, polymer matrix composites, ceramic matrix composites. The several types of reinforcements are glass fibers, ceramic particles, metallic glasses [1]. The composite material where the matrix is metal and the other material may be either metal or any other material is called as metal matrix composites [2]. Composites have several applications and are used in the manufacture of variety of products such as car bodies, spacecraft wings, engine components, missiles, tennis rackets etc. The surface between the matrix phase and the reinforcing phase is called interface. Interface is a boundary through which the different properties of the materials such as elastic modulus, density, and concentration change, etc change. The interface plays a vital role in determining the mechanical properties of the composite. This is because of the large surface area occupied by the interface. Therefore the interface between the matrix and the reinforcement plays a crucial role in determining the resultant properties of the composite and the strength of the composite depends on the strength of the interface [1].

2. Computational method

MD simulations of tensile and shear have been carried out using well tested and widely used LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) code [3]. EAM-FS (Embedded Atom Model Finnis-Sinclair) potential is used for modeling the interactions between Cu and Zr atoms. In Finnis/Sinclair model total energy of an atom is represented by the following equation [4].

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_{\alpha, \beta}(r_{i,j}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha, \beta}(r_{i,j})$$

where F is the embedding energy which is a function of the atomic electron density ρ , ϕ is a pair potential interaction, and α and β are the element types of atoms i and j . The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbors j of atom i within the cutoff distance. Fig.1 shows the model Cu-Cu₅₀Zr₅₀ interface. The simulation parameters are as follows

Simulation parameters:

- Box size: 100 Å (x) × 110 Å (y) × 50 Å (z) comprising of ~37000 atoms
- Ensemble: nvt
- Boundary conditions: S S S for mode-I and S S P for mode-II

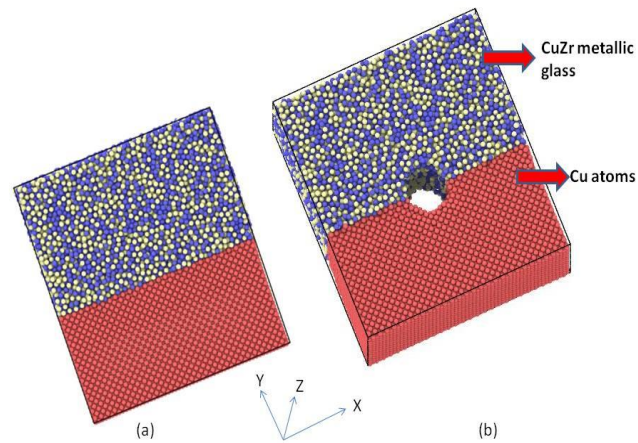


Fig.1 Cu-Cu₅₀Zr₅₀ model interface: a) without crack b) with crack

3. Results and Discussions

Fig. 2 shows the stress-strain curves and the corresponding atomic position snap shots of the interface subjected to mode-I and mode-II loading conditions at different strain rates and temperatures. It is observed that all the stress-strain curves show a linear elastic behavior followed by a drop in the stress indicating plastic deformation. Plastic deformation occurs by slip as evident from the atomic position snap shots. The maximum stress increases with increase in strain rate and decreases with increase in temperature. In the mode-I type of loading the interface separation occurs by initiation of voids at the interface (Fig. 2a). In the sample with crack at the interface the separation occurs by expansion of the crack (Fig. 2c). In the mode-II type of loading the interface strength is found to decrease with increasing temperature. The drop in the stress indicating plastic deformation occurs by slip. In the presence of crack the stress is found to be less as this acts as a source of dislocations.

(a)

(b)

(c)

(d)

Fig. 2 : stress-strain curves and the corresponding atomic position snap shots of the interface subjected to mode-I (a, c) and mode-II loading (b, d) conditions at different strain rates and temperatures.

4. Conclusions

- ❑ Tensile as well as shear strength decrease with increase in temperature and increase with strain rate.
- ❑ The presence of crack decreases the strength of the interface. The crack expands and results in fracture of the samples.
- ❑ Fracture in mode-I deformation occurs by formation of voids at the interface. Crack closure occurs during mode-II type of deformation.

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References

- [1] Chawla, Krishan K. Composite materials: science and engineering. Springer Science & Business Media, 2012.
- [2] Callister, William D., and David G. Rethwisch. Materials science and engineering: an introduction. Vol. 7. New York: Wiley, 2007.
- [3] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J Comp Phys, 117, 1-19 (1995)
- [4] Dai, X. D., et al. "Extended Finnis–Sinclair potential for bcc and fcc metals and alloys." Journal of Physics: Condensed Matter 18.19 (2006): 4527.