ATOMISTIC INVESTIGATION OF ENHANCED TENSILE DUCTILITY OF METALLIC GLASS MATRIX COMPOSITE WITH CRYSTALLINE SECOND PHASE

Shaoxing Qu[a] & Haofei Zhou
Department of Engineering Mechanics, Zhejiang University, Hangzhou 310027 China

Summary Atomistic simulations are performed to investigate the effect of nanoscale crystals on the mechanical response of a $Cu_{50}Zr_{50}$ MG. By carefully designing the patterns of the crystalline second phases embedded in the MG matrix, we have developed a toughening strategy capable of achieving a ductility increase of about 7% compared with pure MGs. Shear band propagation is found to be effectively arrested by the crystals, resulting in the formation of a shear band network in the MG matrix.

INTRODUCTION

MGs possess unique mechanical properties such as high strength, large elastic limit, and high fracture toughness. In their bulk forms, however, MGs exhibit poor ductility due to the intrinsic lack of strain hardening mechanisms. The concept of MG matrix composites (MGMCs) has been raised to achieve optimized mechanical properties, especially improved tensile ductility, in BMGs. In general, the composite is composed of a crystalline second phase (in the form of nanocrystals, dendrites, or fibers) embedded in a MG matrix. By matching fundamental mechanical and microstructural length scales, titanium-zirconium-based BMG composites have recently been synthesized, exhibiting significant room-temperature tensile ductility exceeding 10% and high yield strengths of 1.2-1.5GPa [1]. It is speculated that the characteristic length scales of the composites are extremely important in promoting shear band initiation and suppressing shear band propagation. However, it remains difficult to capture shear band evolution in experiments and thus impossible to correlate the measured mechanical properties with discrete plastic events at small length scales. It is thus worthwhile to conduct atomistic simulations to gain further insights into the deformation mechanisms of MGMCs. We show that, by designing patterns of nanocrystals in MGMCs, shear bands in the MG matrix can be arrested at crystal/glass interfaces. Though mechanisms of shear band branching, reflection, and penetration through crystals, a shear band network is finally formed in the highly deformed MGMC structure. It is observed that the propagation of a few major shear bands, which is the reason for fracture in pure BMGs, is greatly suppressed. By analyzing the stress-strain curves, we also show that shear band softening can be delayed and strain hardening can be achieved in the MGMCs.

METHODS

To systematically study the mechanical behaviour of MGMC structures, we have considered a series of samples covering various shapes, crystalline orientation, and volume fractions of the embedded nanocrystals. For example, Fig. 1 shows three different MGMC samples containing various shapes of nanocrystals. Here, *b* indicates the length of the nanocrystal, while *h* represents the spacing between two nanocrystals along the direction parallel to their long axes. The ratio *b/h* thus defines the shape of the nanocrystals. The colour scheme adopted in Fig. 1 is as follows: Glass atoms are coloured blue, while crystalline atoms are coloured grey. Atoms at crystal/glass interfaces or free surfaces are all coloured green. Each sample consists of about 2,500,000 atoms and possesses a dimension of about $78.6 \times 84.2 \times 5.6$ nm^3. Samples with smaller dimensions, i.e. $40 \times 42 \times 5.6$ nm^3, and larger dimensions, i.e. $107 \times 118 \times 5.6$ nm^3, are also considered to study size effect.

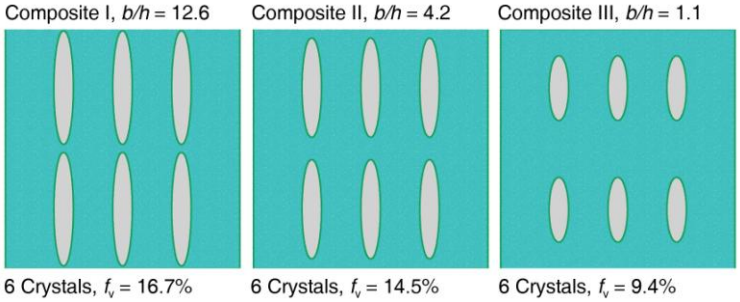

Figure 1 Three different MGMC structures considering shape effect of the embedded nanocrystals. The ratio *b/h* defines the shape of nanocrystals, while f_v is their volume fractions in the composite structure.

Atomic interactions are described by embedded atom method potentials for both MG atoms and crystalline atoms [2,3]. To construct composite samples as shown in Fig. 1, MG samples are initially prepared by using a melting-quenching procedure, and then inserted with nanocrystals of specified patterns. The entire system is relaxed for 1 ns with a timestep of 1 fs before uniaxial tension loading with a strain rate of 1×10^8/s. For the composite structures shown in Fig. 1, external loading is applied parallel to the long axis of the nanocrystals. Temperature and pressure are maintained at 50 K

[a] Corresponding author. Email: squ@zju.edu.cn.

and zero during loading process. Periodic boundary conditions are applied to all directions except for the one with free surfaces.

RESULTS AND DISCUSSION

In pure MGs, shear bands are observed to traverse the entire sample with an angle of ~45° relative to the loading direction, causing shear band steps at the free surfaces. Inhomogeneous plastic deformation is highly localized in these major shear bands. Fracture is not observed due to the small size of our system. In composite MGs, shear bands are frequently arrested before propagating further into the matrix. It is observed that the MG matrix is subdivided by the nanocrystals into smaller domains where shear band propagation can be confined by the crystal/glass interfaces. Besides shear band blocking, reflection of shear bands is also observed nearby nanocrystals in our simulations. The penetration of a shear band through a nanocrystal is available, causing dislocation gliding and formation of stacking faults in the crystal. The shear band also changes its propagation pathway after its penetration. These mechanisms imply that, in MGMC structures, plastic deformation distribution is managed by the interactions between crystals and MG matrix. In our simulations, a shear band network with a homogeneous distribution of plastic deformation is observed in MGMC structures, which is a result of operation of these mechanisms.

To examine the toughening effect of second-phase crystals, stress-strain curves and normalized number of STZ atoms for the composite samples shown in Fig. 1 are plotted in Fig. 2. It is seen that the pure MG sample softens quickly at a strain of ~10% due to unconfined shear banding. As the shape of the nanocrystals changes, the stress drop on the curves are delayed, representing suppression of shear banding in these composite structures. For the composite sample with b/h = 12.6, shear band softening is postponed until a strain of ~17%, gaining an increase in plastic strain of ~7%.

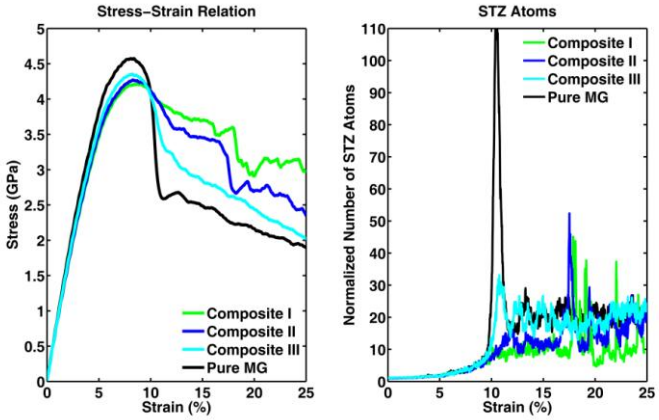

Figure 2 Stress-strain curves and normalized number of STZ atoms for composite samples shown in Fig. 1.

CONCLUSIONS

By performing large-scale atomistic simulations on MGMC samples embedded with various patterns of nanocrystals, we are able to investigate the toughening mechanisms of second-phase crystals and the mechanical response of these composite structures. Our simulations show that homogeneous plastic deformation and enhanced tensile ductility can be achieved by introducing high densities of nanocrystals with a long and narrow shape into the MG matrix. Meanwhile, to effectively arrest shear band propagation, the orientation of these nanocrystalline patterns should be parallel or perpendicular to the external loading force. The obtained toughening effect is more significant in composite samples with larger dimensions, which means our toughening strategy is applicable in real conditions. It is also found that shear banding in the MG matrix can be confined by crystal/glass interfaces, which finally leads to a network of minor shear bands. This explains the enhanced tensile ductility and shed insights on the underlying deformation mechanism in MGMC structures.

References

[1] Hofmann D. C., Suh J. Y., Wiest A., Duan G., Lind M. L., Demetriou M. D., Johnson W. L.: Designing metallic glass matrix composites with high toughness and tensile ductility. *Nature* **451**:1085-1089, 2008.

[2] Mendelev M. I., Rehbein D. K., Ott R. T., Kramer M. J., Sordelet D. J.: Computer simulation and experimental study of elastic properties of amorphous Cu-Zr alloys. *J Appl. Phys.* **102**:093518, 2007.

[3] Mishin Y., Mehl M. J., Papaconstantopoulos D. A., Voter A. F., Kress J. D.: Cu-Mishin1-Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations. *Phys. Rev. B* **63**:224106, 200