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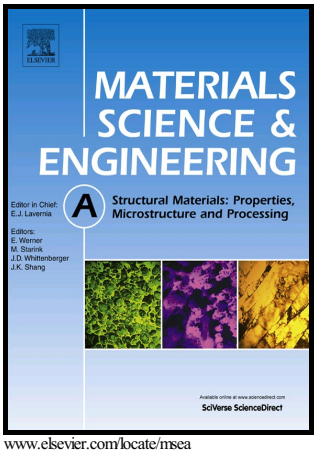

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Dynamical Mechanical Analysis of metallic glass with and without miscibility gap

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Abstract

The dynamic mechanical properties of the miscible $Cu_{50}Zr_{50}$ and immiscible $Cu_{50}Ag_{50}$ amorphous materials are investigated to explore the relationship between deformation mechanism and relaxation of glass through molecular dynamics simulation with modified embedded atom method (MEAM). It is found that the mechanical hysteresis of $Cu_{50}Ag_{50}$ glass is more pronounced than that of $Cu_{50}Zr_{50}$ glass. The storage modulus decreases with increasing loading period or amplitude; while the loss modulus increases till the maximum, corresponding to the beginning of α −relaxation. The β −relaxation in both $Cu_{50}Zr_{50}$ and $Cu_{50}Ag_{50}$ glass shows excess tails in the loss modulus curves. However, the peak height on the left part in the curve of loss modulus as a function of temperature for $Cu_{50}Ag_{50}$ glass is higher than that for $Cu_{50}Zr_{50}$ system, which indicates that β − relaxation in $Cu_{50}Ag_{50}$ glass is more likely to be activated than that in $Cu_{50}Zr_{50}$ system due to lower number of icosahedra-like clusters. The primary α −relaxation always takes place when the most probable atomic displacement reaches a critical fraction (～23%) for $Cu_{50}Zr_{50}$ and (～21%) for $Cu_{50}Ag_{50}$ of the average interatomic distance, irrespective of whether the relaxation is induced by temperature (linear response) or by mechanical strain (nonlinear).The fast atom is defined by the atom motion displacement to explore the dynamical heterogeneity of the glass. We find that the internal fraction shows linear with the number of fast atom.

Keywords: Metallic glass; Miscibility gap; Dynamical mechanical analysis; Molecular dynamics

1. Introduction

The relaxation and plastic deformation and of metallic glass (MG) are determined by its intrinsic structural heterogeneity. The models such as free volume, flow unit, local fivefold symmetry (LFFS) based on voronoi polyhedron analysis, and local soft modules are used to

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