Thermomechanical behaviour of CuZr metallic glasses under cyclic shear

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Abstract

We perform molecular dynamics simulations of Zr50Cu50 metallic glass samples submitted to mechanical deformation. The model consists of two samples of 4800 and 145200 atoms with dimensions of 80x41x24 Aˆ3 and 427x226x24 Aˆ3 respectively. All simulations were carried out using LAMMPS software and particles interact via the modified embedded-atom method potential. Three target temperatures were considered 10, 100 and 300 K and three global strain rates of 10ˆ8, 10ˆ9 and 10ˆ10 s-1 were applied to perform successive deformation cycles.

The simultaneous measurements of the stress-strain curve, and of the temperature evolution during the cyclic mechanical load, are used to determine the thermo-mechanical constitutive laws at the continuum scale. It is shown that a finite strain rate induces simultaneous irreversible rearrangements and collective effects at the atomic scale, giving rise to memory effects in temperature rises that can reach few tens of degrees in plastic zones. Finally, the macroscopic parameters obtained at the continuum scale are compared to local measurements.

Keywords: metallic glasses, mechanical properties, constitutive laws

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