Atomistic Study of the Mechanical Properties of a Sintered Bulk Metallic Glass (Nanoglass)

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ABSTRACT

Metallic glasses with porosity have been on the spotlight in recent years, and much research has been done on them [1-2], in an effort to improve the understanding of the mechanics of deformation. The behavior of the material in the elastoplastic regime may be controlled by the introduction of pores, thus the interest on simulating them.

Large deformation is normally a consequence of shear transformations zones (STZ) collapsing into shear bands (SB) which may lead to catastrophic failure. It is widely known that in crystalline metals the addition of nanopores slows down dislocation motion and changes the resulting plastic deformation. Similarly, pores in metallic glasses limit the propagation of shear bands and allow a more homogeneous deformation.

In previous work [3] we determined constitutive parameters of the $Cu_{46}Zr_{54}$ metallic glass as a function of temperature. We will now present results for a metallic glass with the same composition, but fabricated by sintering of BMG nanoparticles, which results in samples with porosity, similar to "nanoglass" samples in some experiments and simulations [4-5]. Atomistic simulations are carried out using Molecular Dynamics (MD), and analysis includes atomic Voronoi polyhedra, and atomic stress and strain tensors. We analyse the dependence of deformation on solid volume fraction, and the way deformation is distributed throughout the sample, as a function of initial porosity.

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