Molecular Dynamics Simulations of Nanoglasses

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Fig. 1: Microstructure of metallic NGs. Glassy grains are shown with the blue color and glass-glass interfaces with yellow color.

Introduction

Metallic glasses (MGs) are of great technological interest because of their high strength and hardness [1]. However, when MGs are exposed to an external load then they fail catastrophically along a single shear band [2]. On a microscopic scale, shear bands in MGs are considered to be controlled by the activation of shear transformation zones that represents local shearing of approximately 100 atoms [3]. To avoid the catastrophic failure in MGs and improve their ductility, predeformed samples and glasses with nanocrystalline inclusions have been studied in the past [3,4]. The main findings of these studies is that the presence of such microstructural inhomogeneities in the samples prevent the formation of the shear band, which could cause catastrophic failure. Recently, a new class of MGs have been proposed, the so-called metallic nanoglasses (NGs) [5]. Metallic NGs have been produced by consolidating nanometer-sized glassy spheres which are prepared by inert-gas condensation [5,6] (Fig. 1). Recent experimental studies have shown that metallic NGs present enhanced ductility [5] and ferromagnetism [7] when compared with MGs. In addition, NGs are promising candidates as materials for medical applications [8].

Methods

The properties of materials are strongly controlled by their microstructure. Despite the improved properties of NGs, their microstructure is not well understood. Atomistic simulations are
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useful tools to gain insights on the atomic level into the structure of a material. Several microstructural models for NGs have been proposed based on atomistic simulations. Although those models have offered explanations on the origin of enhanced ductility in NGs, a proper structural model which could explain the experimental observations on the structure of NGs is still lacking. We have performed large-scale molecular dynamics simulations, as implemented in the LAMMPS software [9], to investigate the microstructure of the NGs.

Results
Our results reveal that NGs are amorphous materials with inhomogeneous microstructure which consists of glassy grains connected with glass-glass interfaces (Figure). Structural analysis show that the glass-glass interfaces in NGs are characterized by a lack of short range order compared to MGs and a width of about 1 nm. In addition, they have a different composition than the glassy grains. The present microstructure for NGs is consistent with experimental analysis by means of small-angle X-ray scattering measurements and element mapping data on the Sc-Fe Ngs [5].

Outlook
In the future, we plan to perform molecular dynamics simulations to study the deformation mechanisms in NGs. It is proposed that the glass-glass interfaces prevent strain localization. We will perform a set of mechanical tests in order to get better understanding on how glass-glass interfaces in NGs influence their mechanical properties.

Reference

Last Update: 2020-03-12 16:02