Enhancing the ductility of bulk metallic glasses: an approach by atomistic simulations

Context:

Bulk metallic glasses (BMG) have remarkable structural and mechanical properties due to the absence of long-range order: high toughness, exceptional mechanical strength, elastic deformation almost ten times larger than their crystalline counterparts, which has made them a subject of study since the 90s for their potential structural and industrial applications (for micromechanics, jewelry and biomaterials). On the other hand, the Achilles heel of these materials for engineering applications is the low ductility at room temperature. As a clear structural description of the BMG is still absent, their deformation mechanisms are far from being understood. To better understand the physical and structural mechanisms underlying the mechanical behavior of BMG, it is necessary to analyze the factors that influence the elastic and plastic deformation of these amorphous materials. Although experimental techniques have been developed to progress in the field, these methods often have limitations due to the extreme fragility of the glasses and the difficulty to visualize the atomic rearrangements responsible for the observed behavior. For this reason, given the enormous development of the computing power in recent years, numerical simulation approaches, especially Molecular Dynamics approach, are increasingly used to easily access the atomic scale and analyse the local dynamical movements that are responsible for the mechanical behavior in the elastic and plastic regime. This approach will be pursued in the proposed thesis in order to better establish a link between the local atomic dynamics, the material microstructure and the observed mechanical properties.

Topic and objectives:

This thesis project is in line with three previous PhD projects carried out at MATEIS laboratory at INSA Lyon, in the framework of the CSC program: the first is an experimental work done by Jichao Qiao (now Professor at Xi'an University), the second a numerical and experimental thesis by Guojian Lyu (now post-doc researcher at the Chinese Academy of science in Beijing), the third by Meng Liang (still in progress). In the PhD work of M. Liang we have established a framework to investigate the atomic-scale plasticity of BMG. In this PhD thesis we will extend this approach to BMG submitted to mechanical and thermal pre-treatment in order to understand the signature of rejuvenation on the small-scale plasticity.

The aim of this project is to simulate the mechanical behavior of BMG in the elastic and plastic regime, using Molecular Dynamics (MD) techniques to identify the physically relevant mechanisms of plasticity at the molecular scale and to assess under which conditions the system can be rejuvenated in order to enhance its ductility. Based on recent experimental works proposing to improve ductility by applying thermal cycles at very small temperatures or by elastostatic loading of the sample, the PhD thesis will focus on the following objectives:

1) Perform and analyze MD simulations for a BMG submitted to a thermal cycle and conclude about the parameters and the mechanisms responsible for rejuvenation.
2) Perform a parametric study of the effect of different mechanical pre-treatments (static loading, cyclic loading) on the mechanical behavior of BMG to see under which conditions rejuvenation can be obtained.
3) Analyze the small-scale plasticity of the simulated systems by using an ad-hoc algorithm that we have recently developed in collaboration with Tristan Albaret (Professor at Lyon 1 University) in order to link the observations of points 1 and 2 to the atomic-scale dynamics.

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