Intrinsic and extrinsic size in metallic glasses

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Chapter 7

Summary and outlook

7.1 Summary

Investigation of the mechanical behavior of materials is an important key topic in nanoscience and nanotechnology. Most of the nanodevices fail due to (thermo)mechanical processes and therefore fundamental questions about size effects in these nano-objects are very relevant. Also, mechanical testing at larger scales differs significantly differ from testing at smaller specimens and therefore size effects open a new potentially interesting area for investigations.

A metallic glass (MG) represents an exceptional class of materials which possesses rather unique properties for metals. It allows producing of large amount of stresses within the specimen, but it lacks the plasticity and undergoes shear band deformation rapidly. Therefore investigations of size effects in metallic glasses plays important role. The recent developments of nano- and microscale manufacturing processing techniques using e.g. focused ion beam or electron beam have significantly increased the importance of materials with homogeneous structures (Chapter 2). By applying FIB-based techniques, various specimens with smooth surfaces on a nanometer scale can be fabricated from MGs. Chapter 3 presents new in-house developed methods for the preparation of nanopillars, which enable to avoid FIB milling artifacts such as tapering and redeposition.

Size effects can be grouped into intrinsic or extrinsic. Intrinsic size effects are commonly controlled by the inner structure and materials processing. In MGs, they are represented by the collective behavior of(shear transformation zone) STZs (discussed in chapters 3 and 5). In-situ quantitative compression tests which revealed intrinsic and strong size effects of taper-free metallic glass nanopillars inside a transmission electron microscope (TEM) on different MG compositions show predominantly an inhomogeneous and intermittent plastic flow characterized by shear banding events. The deformation is defect-nucleation-controlled in larger pillars but becomes propagation-controlled in smaller pillars. Pillars with a diameter smaller than a certain diameter show a homogeneous flow behavior without shear banding during compression.

The initial structure and chemical composition of MGs also affect the deformation behavior at the nanoscale (Chapter 4). MG pillars of different alloy systems and compositions, Cu-based, Al-based, Zr-based alloys showed the shift in transition threshold depending on the bulk modulus and Poisson's ratio which also were affecting the deformation mode and ductility of MGs at the nanoscale. Higher values of Poisson's ratio, and consequently lower values of the μ/B ratio of MG composition, lead to a more ductile behavior. The $Al_{86}Ni_9Y_5$ taper-free metallic glass showed the highest transition threshold for brittle behavior, i.e. above pillar diameter of 300 nm (discussed in Chapter 5).

In accordance with our predictions $Al_{86}Ni_9Y_5$ MG shows plastic deformation becoming even more apparent through softening and toughening effects. These phenomena are revealed and characterized through the cyclic micro- and nanopillar tests. The proposed experimental technique of loading and unloading cycles is capable of determining the mechanical performance in metallic glasses, and opens a new route to the characterization of the deformation behavior of metallic glasses down to 100nm sizes.

Extrinsic size effects as opposite to intrinsic are caused by dimensional constraints due to preparation methods or influence of preparation technique on the sample during or before mechanical testing. These extrinsic constraints arise due to geometry of the specimens, aspect ratio or they are influenced by the FIB interface layer. The pillar aspect ratio has a large influence on deformation behavior representing a clear extrinsic size effect. Very high strains and ductility were achieved in bending at high aspect ratios, which reveals a possibility for future application developments with MGs.

Interactions between intrinsic and extrinsic size effects in MGs are particularly interesting, although the current understanding of this topic is limited. As argued in Chapter 3, tapering is a serious problem in investigating the deformation behavior of micro-pillars under compression. Tensile experiments were performed in order to separate the difference between extrinsic and intrinsic size effects (Chapter 6). The transition threshold from inhomogeneous flow which is characterized by shear banding events is shifting compare to compression experiments towards a lower diameter of the specimens. It indicates the separation of volumetric extrinsic size effect which was concluded by compression experiments and intrinsic size effects on MG composition which is related to collective behavior of STZs.

7.2 Outlook

Based on the tensile experiments on $Al_{86}Ni_9Y_5$ and $Zr_{61.8}Cu_{18}Ni_{10.2}Al_{10}$ MG samples many questions about the mechanical behavior of MGs at nanoscale could be properly addresses. The change in deformation behavior from brittle fracture to necking starts at samples in tension at smaller diameters in comparison to the compression. The influence of chemical composition on the transition threshold for both regimes was also observed. It confirms our predictions about volumetric size effect of MGs at nano-scale and can be explained by the competition between the nucleation and propagation of STZs at different stress fields and volumes.

Despite of the constant yield stress in compression, tensile experiments show unique increase in strength. Strain hardening was observed for smaller sample sizes in tension. However tensile experiments at the smallest scale revealed the influence of FIB ion irradiation on specimens and suggest that it plays also a role in appearance of extrinsic size effects of MGs in tension.

From a theoretical viewpoint an interesting question to address is the influence of statistics. In crystalline materials the stress-strain response of micropillars during compression is characterized by significant stochastic effects, which are manifested through multiple strain bursts [1,2,3,4]. The stress-strain curves for same diameter pillars differ significantly, however, they can be enclosed within bounds, and therefore a size effect is noted. Recently it has been shown that the stochastic effects observed in the stress-strain behavior of both crystalline and glassy micropillars are successfully captured by implementing a gradient formulation in a cellular automaton and using a stochastic term to characterize the yield stress [5,6,7] . The numerical code was able to interpret the stochastic stress-drops observed during nanopillar compression and the observed size-dependent strengthening as well. In particular for glassy materials, having a proposed internal self-averaging structure when no mechanical stress is applied, this approach dealing with stochastic effects is worthy to examine in further detail.

The term size effect is used to distinguish all the cases when materials change the properties by reducing the dimensions of the specimen. Nowadays, material technologies emphasize miniaturization. Nano-system fabrication and developments are a very interesting and challenging field of scientific research bridging microelectronic, physics, chemistry, mechanics. Recent progresses have allowed highly integrated and high-performance micro- and nano- electromehanical devices and the further development of such systems depends critically on the choice of appropriate materials. In this regard, properties of metallic glasses at nanoscale are providing a significant and unique potential. Understanding mechanical properties of MGs at nanoscale is therefore a high impact issue of material research. The investigations on different compositions in tension and in compression should be addressed. With respect to the sizes it is interesting also to reveal the influence of initial MG structure and temperature treatments on the transition thresholds. In summary, potential applications of this research are feasible and it offers a bright prospective for future work in materials science.

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List of publications

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7. O.V. Kuzmin, Y.T. Pei and J.Th.M. De Hosson, Fabrication method of nanopillars through focused ion beam cutting, (submitted).
8. O.V. Kuzmin, Y.T. Pei and J.Th.M. De Hosson, Size effects of MGs at nanoscale in tension, (in preparation).