Experimental report

09/02/2016

Proposal: **6-05-946**

Council: 4/2014

Title: Atomic Dynamics of Bulk Metallic Glasses under Tensile Stress

Research area: Materials

This proposal is a continuation of 6-05-912

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Samples: PdCuSi

Instrument	Requested days	Allocated days	From	To
IN6	6	4	20/11/2014	24/11/2014

Abstract:

In the application of bulk metallic glasses (BMG) their mechanical properties are the most important. They show an extreme strength at ambient temperature but fail abruptly when yield sets in, which strongly limits their applications. This phenomenon is related to their disordered inhomegeneous structure, consisting of soft regions, in which the instability is initiated, and a network of hard regions surrounding these softer shear transformation zones (STZ). The collective rearrangement of the atoms in the STZ under load will be reflected in the atomic dynamics, especially in the low energy modes, as the origin of the glass-characteristic low energy modes is most likely in these more loosely packed regions (free volume) as well. We want to investigate the atomic dynamics, while our sample is stressed below the yield point, to look for any changes in the generalized vibrational density-of-states with applied stress and especially to search modes indicating the approach of the sudden failing of the material. We want to investigate the connection between the changing mechanical properties and the atomic dynamics of the BMG.

Report on experiment 6-05-946

Atomic Dynamics of Bulk Metallic Glasses under Tensile Stress

Slow cooled metallic glasses have attracted much interest in recent years because of their favourable mechanical and chemical properties. Their exceptional hardness and strength makes them favourable materials in applications. The main drawback in their use is their glass-like sudden catastrophic yield under (too high) load, which limits their very favourable mechanical application [1,2]. The reason for this handicap in their use is most likely their heterogeneous atomic structure, which – as far as we know up to now – consists of soft regions surrounded by denser, hard "shells" made up of clusters, often with perfect or partial icosahedral symmetry. The soft regions, often called shear transformation zones (STZ) in context with mechanical properties [3] provide the low energy barriers in cooperative rearrangement of atoms needed in deformations of the glass. In the catastrophic yield under load, these STZ are assumed to connect (like in a percolating network) and form a shear band, which transverses the complete sample: the glass breaks. At the same time these soft regions might well be the origin of the low energy modes, found in metallic glasses [4]. We therefore assumed, that one could find a change of the Generalized Vibrational Density-Of-States (GVDOS), when these soft regions start to deform under mechanical load.

In our very first experiment we did not find any influence in the small load region, which we applied to our samples, but we could show, that even the small amount of sample (2 mm diameter, 30 to 35 mm length) was sufficient to determine a reasonable GVDOS within runs of 24 to 28 h, - and insufficient to determine the dynamic structure factor on IN6. For this we would have to do an experiment on IN5.

Before the experiment 6-05-946 we performed an experiment without neutrons but with the same dilatation gear (to avoid calibration uncertainties), which we than have used in the experiment. From several dilatation experiments, only 3 were properly registered by the very old dilatation gear. One of these result is shown in Fig. 1: a scan from 0 N to 470N (in this experiment without neutrons, the sample used for the experiment shown in Fig.1, had a mean diameter of 3.2 mm, thus the factor in front of the force, i.e. the inverse sample cross-section in m^2, is $12.43\ 10^4$ to get the strain in Pa).

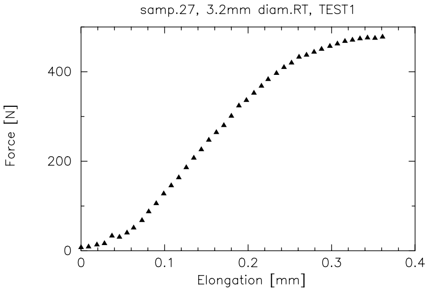

Fig.1 Strain-stress(elongation) curve showing the linear and non-linear stress

As far as we can obtain from this curve, yielding sets in at approximately 330N. With this information we conducted our experiment between 0 and nearly 400N this time. This means that we did 5 sample measurements (plus V-calibration and empty dilatation gear) in the same 4 days, which we had for our first test-experiment, where we measured 2 GVDOS. Consequently our new results have a very significant statistical error (see Fig.2). It is therefore not surprising that we have taken the results from our first test-experiment, when the GVDOS measured at no strain had to be used. To regain the reasonable statistical accuracy, we had in our first test experiment, we will need a longer experiment. Fig. 3 shows one of the final results of this experiment: a clear change of the GVDOS under the stain of 100N already (in the experiment only 1 sample with a mean diameter of 1.57 mm was used, thus the conversion factor to Pa in this case is 12.91 10^4).

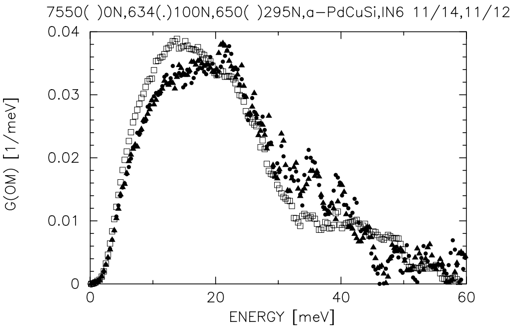

Fig.2 GVDOS of PdCuSi measured at 0N (o) (2012) and 100N (•)(2014)

This result clearly proves, that our assumption, that we might be able to change the atomic vibration in the glass well below the yielding strain, was correct. Surprisingly, at 100N the relaxation process is already finished. As shown in Fig. 3 the differences between all GVDOS measured at higher strains (200, 295 and 387N) and the one measured at 100N fluctuate around 0 in the full energy range of the GVDOS.

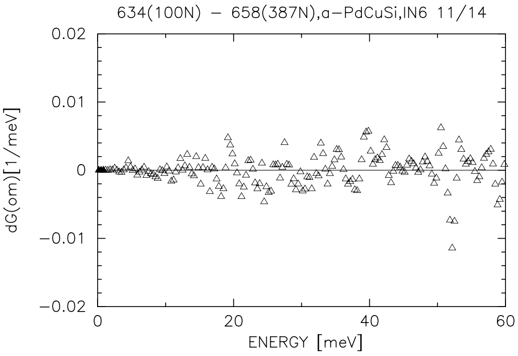

Fig.3 Difference of the GVDOS measured at 387N and 100N

With this new information: the assumed effect exist and it is finished at or below 100N we can now do a careful investigation of the GVDOS of PdCuSi at stresses between 0 and 100N with better statistics than we obtained this time.

We would like to thank Michael Marek Koza and Jerome Halbwachs for their help at the instrument and Thilo Pirling for his help at his dilatation gear.

[1]M.M. Trexler, N.N. Thadhani Progr.Mat.Sci. **55** (10) 759 [2]S. Takeuchi, K. Edagawa Progr.Mat. Sci. **56** (11) 785 [3]C.A. Schuh et al. Nat.Mater. **2** (03) 449 [4] J.-B. Suck et al. J.Phys. C **13** (80) L167