

Proposal:	6-05-912	Council:	4/2012	
Title:	Atomic dynamics of bulk metallic glasses under tensil stress			
This proposal is a new proposal				
Research Area:	Materials			
Main proposer:	SAMWER Konrad			
Experimental Team:	SUCK Jens-Boie			
Local Contact:	KOZA Michael Marek			
Samples:	Bulk metallic glass/Cu46Zr42Al7Y5			
Instrument	Req. Days	All. Days	From	To
IN6	0	4	06/11/2012	12/11/2012
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 limits the 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 between these shear transformation zones (STZ). The collective rearrangement of the atoms in the STZ will be reflected in the atomic dynamics, especially in the low energy modes, the origin of which is most likely in these more losely packed regions (free volume) as well. We want to investigate the atomic dynamics, while our sample is stressed below the yield point, to see any changes with applied stress and especially to look for 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.				

Atomic Dynamics of Bulk Metallic Glasses under Tensile Stress

Slow cooled bulk metallic glasses have become new materials with high interest in their application. The main properties, which have lead to this interest in these structurally disordered alloys, are their mechanical properties, their exceptional hardness and strength. The main drawback in their use is their glass-like, sudden catastrophic yield under (too high) load, which limits drastically their otherwise very favourable mechanical applications [1,2]. The reason for this catastrophic failure (especially under tension) is most likely to be found in the heterogeneous structure of these glasses: soft regions, which provide the low energy barriers in cooperative rearrangement of atoms as needed in relaxational processes [3] and denser, harder “shells” made up of clusters, often with complete or partial icosahedral geometry. In context with the mechanical properties, these soft regions are called shear transformation zones (STZ) [4]. They are thought to be the origin of the sudden yield: under load the STZ connect forming a shear band (SB) which transverses the complete sample and lets the glass break catastrophically. At the same time, these soft, less dense regions should be the origin of the low energy soft modes found in metallic glasses [5]. The assumption that the low energy modes should be influenced, when the soft regions start deforming e.g. under tensile stress, is a plausible one and the starting point of our investigations. While mechanical experiments can come up with the final result of the formation of shear bands, we would like to get information on the beginning of this process.

This first experiment was done on IN6 at room temperature with two very different set- ups to dilate the sample:

A. We used the dilatation gear, borrowed from SALSA, with special clamps to hold the thin PdCuSi-glass stick (2 mm in diameter, $25 \leq l \leq 35$ mm long, this was the longest of our 3 sticks and therefore we used this). As in this first experiment we were too scrupulous, when loading the sample, in order not to break it before the experiment, our requirements concerning the dilatation gear were too low compared to its normal load range, - but will be all right in a next experiment. The load indication therefore was not very reliable. We measured with different, but too low loads, as is shown in figure 1 (numbers are un-calibrated stress indications not N-samples).

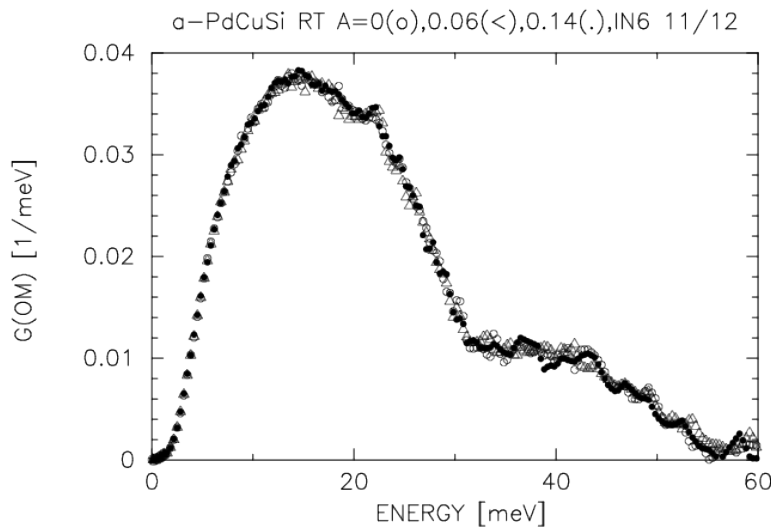


Figure 1: GVDOS of the bulk metallic glass PdCuSi under different tensile stresses below 3N
Indication = 0 (O), 0.06 (Δ), 0.14 (\bullet)

B. We mounted the stick at the top-flange of the scattering chamber and put a weight at the bottom of the sample to create the force we wanted to use. As figure 2 proves this drastic change of sample set-up did not change the obtained results.

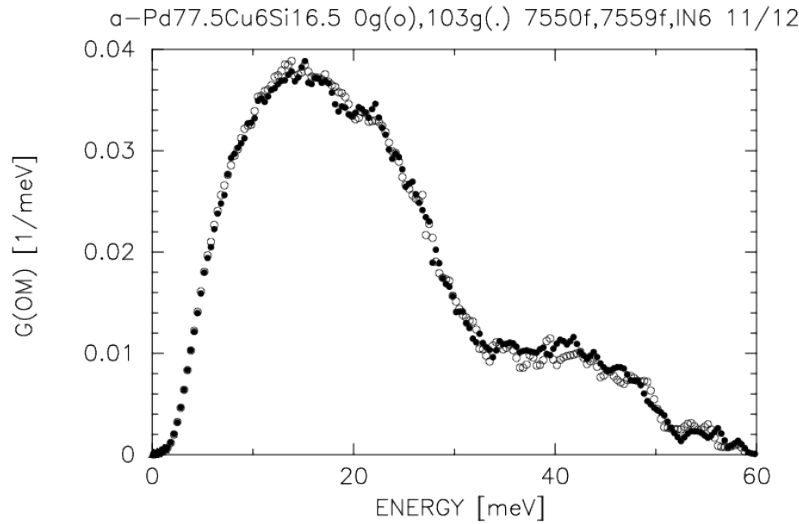


Figure 2: GVDOS of the bulk metallic glass PdCuSi under a tensile stress of 0 (open circles) and 1 N (filled circles). As in fig. 1 no change is observed, especially not in the low energy region, which is measured with good statistical accuracy in this experiment.

At the beginning of this first experiment we had nothing but open questions:

1. At which tensile stress we will see a change of the spectrum?
2. Will this small amount of sample (about 0.05 cm^3 as at least half of the stick-length is needed to fix the stick in the clamps and is covered by Cd), be sufficient to measure spectra with a sufficient statistical accuracy?
3. How sensitive will the results be on the set-up of the experiment, i.e. on the positioning of this match-like object in the IN6 beam?

Even though we still have to answer the most important first question in a future experiment, we are able to give answers to the 2nd and 3rd question:

On IN6 the sample amount is sufficient for a reliable determination of the GVDOS, but not for the determination of $S(Q,\omega)$. For the determination of the total dynamic structure factor we have to use a t-o-f-instrument with an at least a factor 2 to 3 more intense beam at the sample position.

The results obtained are not very sensitive to the experimental set-up as long as the sample is centred with sufficient care. This is everything else but a trivial result as the beam of IN6 is fairly inhomogeneous, being focused on the sample from three different monochromators.

We thank the technician and the instrument responsables of IN6 for their assistance, Dr. Thilo Pirling for his patience while introducing us to the use of his dilatation gear and Richard Ammer for machining part of the sample clamps.

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| [1] M.M. Trexler, N.N. Thadhani, <i>Progr.Mat.Sci.</i> 55 (10) 759 | [2] |
| S. Takeuchi, K. Edagawa, <i>Progr.Mat.Sci.</i> 56 (11) 785 | [3] Q. Hu et al. <i>J.Appl.Phys.</i> 111 (12) 083523 |
| [4] C.A. Schuh et al. <i>Nat. Mater.</i> 2 (03) 449 | [5] J.-B. Suck et al. <i>J.Phys. C</i> 13 (80) L167 |