ESRF	**Experiment title:** Uncovering the nano-scale mechanisms of enhanced plasticity in metallic glasses using inelastic x-ray scattering	**Experiment number**: **MA-3226**
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Shifts:	**Local contact(s)**: Tranh Tra Nguyen	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Zachary Joseph Evenson*

Sandro Szabo*

Rene Bastian Hubek* University of Münster, WWU Germany

Valentina Giordano*

Beatrice Ruta*

Report:

The physical properties of metallic glasses are subject of intense research especially with respect to their mechanical behavior. Recently, it was shown that the mechanical properties of a $Pd_{40}Ni_{40}P_{20}$ metallic glass could be significantly influenced by microalloying of Fe or Co, along with a dramatic influence on the heat capacity excess vibrational modes. (N. Nollmann et al., Scripta Marerialia 111 (2016), 119-122).
Currently running diffusion measurements in our lab revealed for the microalloyed material much faster diffusion paths along the shear bands. Diffusion measurements for the standard composition also showed that, through shear bands caused by deformation, tracer diffusion could be drastically increased (J. Bokeloh, S.V. Divinski, G. Reglitz, G. Wilde, Phys. Rev. Lett. 107 (2011) 235503). Similiar diffusion experiments with the microalloyed material show even faster diffusion rates. The boson peak of deformed samples determined in heat capacity measurements showed an increase in excess phonon modes. For this reason, the interest was present to measure the phonon dispersion using IXS at the beamline ID28 at the ESRF.

The first idea was to measure at very low q-values, in order to investigate the dispersion close to the hydrodynamic limit. For this, half of the first day was used to calibrate for the (12 12 12) setup. The rest of the day the sample was mounted and the elastic S(q) was measured. With this the amorphousness of the sample at the set position was checked. For the night a measurement was started to see if the counts per unit time would be sufficient to measure two samples over the assigned time. With the measured counts per time, an estimation showed that it would only be possible to measure one sample for the entire week. The setup was thus changed to the (9 9 9) crystal orientation, at the expense of a worse resolution. For the (9 9 9) crystal orientation a new calibration setup had to be carried out. After this, a measurement for the ascast PdNiPFe sample was started. One data set can be seen in figure 1. In a first analysis these data were fitted to a 1 mode model.

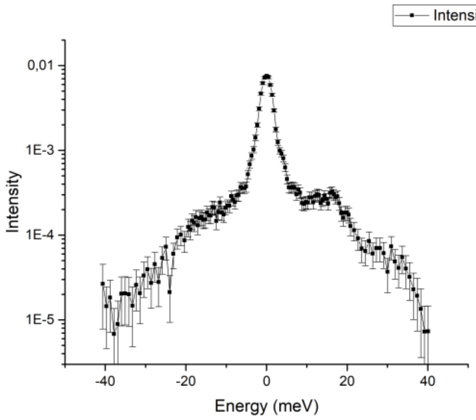

Figure 1: Intensitiy vs. Energy transfer for the PdNiPFe as-cast state.

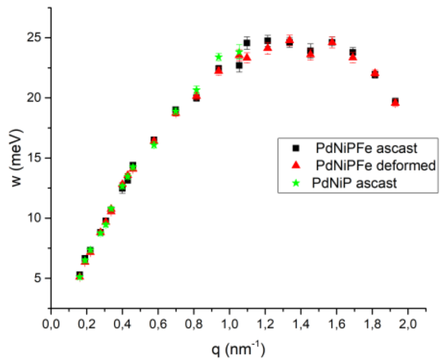

Figure 2: Peak position vs. q. Nearly no influence on the peak position could be observed for deformation or microalloying.

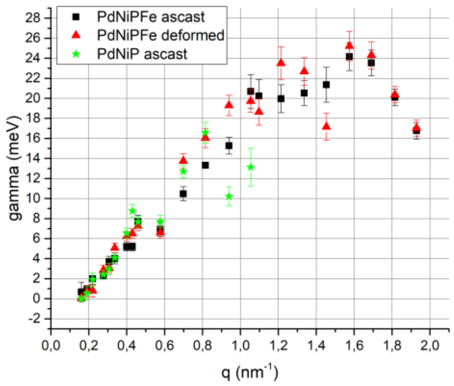

Figure 3: Peak width vs. q. Probably a small decrease of phonon life time is observed through deformation.

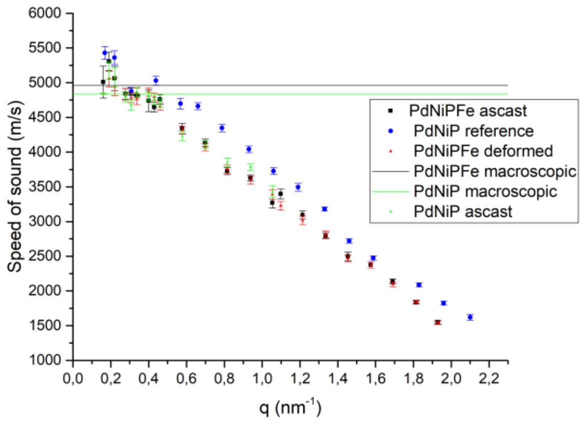

Figure 4: Speed of sound vs. q. The PdNiP reference data are from Hosokawa, Materials Science Forum, 2016.

Next, the deformed PdNiPFe sample was measured. Two measurement configurations were used: with the deformation axis parallel and perpendicular to the scattering plane. For the last experiment, the effect of microalloying was of interest, thus the standard PdNiP composition was measured. A first analysis shows (Figure 2) that the peak position is not influenced by deformation or microalloying, which is rather unexpected. For the peak width (Figure 3) which correlates to the phonon life time, a small influence can be observed. The phonon lifetime of the deformed state is shorter for $0.7 < q < 1\ nm^{-1}$. For low q values the resolution is too low.

Further analysis of the speed of sound (Figure 4) shows nearly no influence of the deformation or microalloying. As one can see, the reference data does not fit within the uncertainty to our measurement. As they do not give any information on actual composition of their material, it could be due to stoichiometry differences. This effect seems plausible, as the difference in measured macroscopic sound velocities is around 100 m/s, which indicates that the composition of the analyzed material may be different.

We referred to several physical properties, like heat capacity and diffusion, where microalloying and deformation showed a significant influence. The IXS measurements showed nearly no influence, which was rather unexpected. A small influence could be observed in the phonon lifetime at high q, which remains to be understood. Further data analysis will have to be done, incorporating different models for the inelastic spectrum. We with to point out here though, that the absence of a detectable influence of microalloying and deformation in these exeriments is a result in itself, and quite unexpected considering that macroscopic properties show drastic changes. In order to clarify the existence of any effect on phonons, we will perhaps need to measure samples where an effect on macroscopic properties is stronger. Measurements of samples under deformation, with the use of a on-line tensile device would also be of interest.