Local mobility and atomic structure in Pd- and Zr-based bulk metallic glasses

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Background incl. aims
Metallic glasses are a category of materials not completely understood yet. Especially the glass transition mechanisms and the origin of structure-property relations are unclear and gaining deeper insights is of great interest. With a detailed analysis of the local structure and atomic mobility in two model systems of bulk metallic glasses, the possibility of observing atomic processes that govern basic glassy mechanisms can be sought after.

Methods
The here investigated Pd- and Zr-based materials are model glass systems with high kinetic stability and superior mechanical properties, respectively. They are prepared by copper mould casting and verified for their amorphous phase by X-ray diffraction. Further characterisation in terms of thermal properties is done by differential scanning calorimetry. Microstructural investigations are based on electron microscopy techniques: In TEM mode, the method of Electron Correlation Microscopy (ECM) is used to probe the local dynamics and structural relaxation times of Pd- and Zr-based metallic glasses. ECM gives further insights into the underlying mechanisms of amorphous phases with nanometer spatial resolution. Experiments are performed both at room temperature and elevated temperatures using FIB-prepared lamella with a Protochips Fusion AX in situ heating holder. Complementary structural investigations concerning the medium range order (MRO) in glassy metals are performed by 4D-STEM fluctuation electron microscopy (FEM), evaluating the normalized variance of speckles in nanobeam diffraction patterns.

Results
ECM yields a structural relaxation time and a stretching exponent from fits to intensity correlations of dark-field images over time. The structural relaxation time is a measure of local mobility in the material and was found to be different for the two investigated material systems, attributed to their different compositions. In addition, the two material systems react differently to the electron beam during the ECM measurements, where the determined stretching exponent might help to understand the underlying dynamics mechanisms in more detail. Comparisons of ECM-determined parameters from room temperature experiments and measurements at elevated temperatures also show a difference between the two material systems, which are connected to the thermal stabilities of each metallic glass. Moreover, the MRO investigated by fluctuation electron microscopy shows different MRO sizes and volume fractions for the two material systems. A comparison of these findings with thermal parameters resulting from macroscopic measurements is performed.

Conclusion
The conducted investigations show clear differences between the two material systems in the local dynamics as well as the atomic structure. These deeper microstructural insights from electron microscopy measurements at various, also elevated temperatures complement the results of macroscopically averaging methods of thermal and mechanical investigations. Combining the findings allows to better understand the glassy state and beam-induced dynamics including underlying mechanisms.

Keywords:

Metallic Glass, Structural Relaxation, ECM