EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

	Experiment title: Tuning the Invar effect in Fe-based bulk metallic glasses by pressure-induced polyamorphism	**Experiment number**: HC 5050
Beamline: BM23	**Date of experiment**: from: 20/09/2022 to: 26/09/2022	**Date of report**: 23/02/2023
Shifts: 18	**Local contact(s)**: Angelika Rosa	*Received at ESRF:*

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Report:

It is known that ferromagnetic Fe-based bulk metallic glasses (BMGs) universally show an anomalously low coefficient of thermal expansion below their Curie temperature T_C. This effect is known as the Invar effect and rarely seen in crystalline materials, with Fe-Ni around 36 at% Ni being a notable exception. The Invar effect in BMGs is inherently linked to the amorphous atomic arrangement because the it is not present anymore after the BMGs have crystallized. The volume transformations of the Invar effect are fully reversible around T_C. It is assumed that the Invar effect originates from the co-existence of multiple local arrangements (primarily of Fe) that differ in both their volume and magnetic properties. By applying high pressure in a diamond anvil cell (DAC) the dense local arrangements can be stabilized and their effect on the thermal expansion be studied.

During this beamtime we performed extended X-ray absorption fine structure (EXAFS) experiments on $(Fe_{73.2}B_{22}Y_{4.8})_{95}Mo_5$ at the Fe K-edge. The BMG samples were prepared as flakes from a splat-quenched sample and placed in a resistively heated DAC along with ruby and gold for pressure and temperature calibration. The rhenium gaskets where prepared on-site at ESRF. EXAFS scans were recorded at various temperature-pressure points within the relevant landscape (T = 300 … 700 K, p = 0 … 22 GPa). Due to the pressure hysteresis of the DAC, a new sample was loaded for every temperature and a pressure series was recorded with increasing

pressure. Based on the signal-to-noise ratio multiple EXAFS scans were performed at the same temperature-pressure point and then averaged.

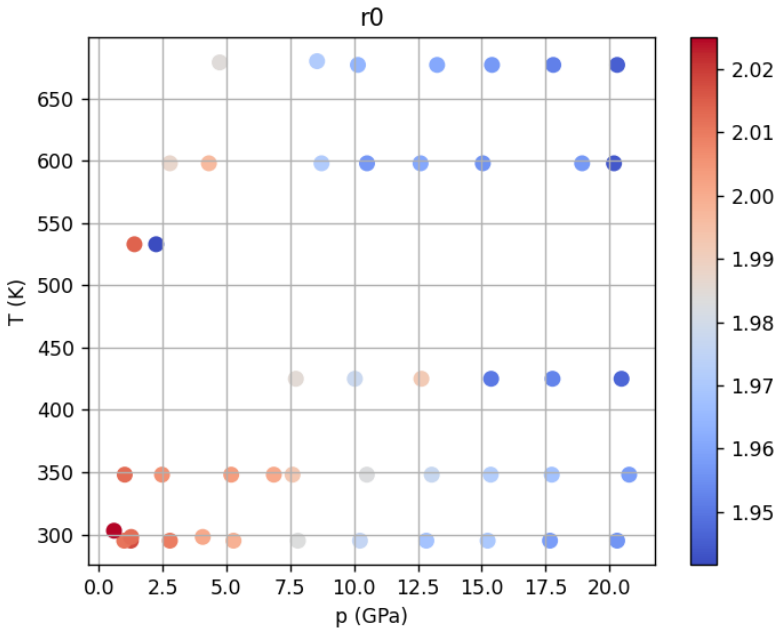

Figure 1: Average bond distance of Fe across the temperature-pressure landscape.

Figure 1 shows the average bond distance r_0 (r_0 temperature scale in Å, not corrected for phase shift) of Fe across the temperature-pressure landscape. The Curie temperature is at 500 K. One can clearly see the effect of pressure which reduces the bond distances significatly at all temperatures. Temperature has the opposite effect but it is much smaller in the studied temperature-pressure range.

Figure 2 shows an exemplary fit to the partial pair correlation function around Fe. The first atomic shell is well described by a Gaussian and is associated with Fe–Fe pairs.

Additionally, a preliminary model based on the EXAFS equation

$$\chi(k) = S_0^2 \sum_j N_j \frac{f_j(k)}{kR_j^2} \exp\left(-\frac{2R_j}{\lambda(k)}\right) \exp\left(-2k^2\sigma_j^2\right) \sin\left(2kR_j + \delta_j(k)\right)$$

could be build which includes pressure and temperature effects. First results indicate that the magnetic interactions help to stabilize the local atomic arrangement. This can help to understand its role in the Invar effect, why it is universal in Fe-based BMGs but rare in crystalline materials and which magnetic interaction are at its origin. A scientific publication is currently in preparation.

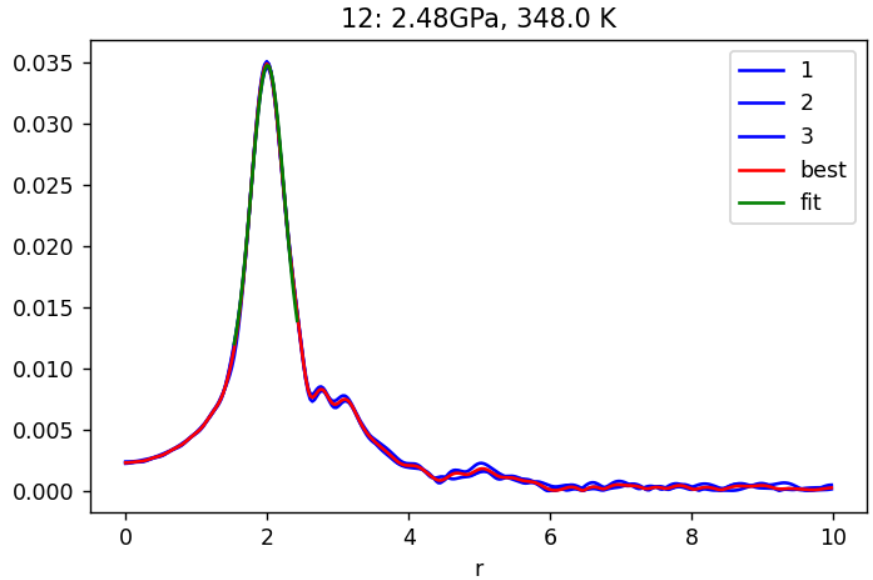

Figure 2: Fit to the partial pair correlation function.