	Experiment title: Optic-like excitations in the metallic glass	**Experiment number**: HD-644
Beamline: ID28	**Date of experiment**: from: 31.10.2012 to: 03.11.2012	**Date of report**:
Shifts: 9	**Local contact(s)**: Alexei BOSSAK, Michael KRISCH	*Received at ESRF:*

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Report:

In this project it was proposed to study by inelastic X-ray scattering (IXS) the high frequency dynamics of $Zr_{50}Be_{50}$ metallic glass within the first pseudo-Brillouin zone. Inelastic neutron scattering (INS) experiment [1] reveals the existence of acoustic- and optic-like excitations in the vicinity of the first peak of static structure factor. However, the inherent to INS kinematic constraints complicate the investigations at small momentum transfers, where the excitations are much more defined.

The lack of any kinematic restrictions for inelastic X-ray scattering would permit us to access of the desired Q-E region. The experiment was performed at room temperature at an incident photon energy of 17794 eV, using the silicon (999) setup, providing an overall energy resolution of 3 meV (FWHM). Spectra for 3 angular settings of the spectrometer arm were recorded, spanning a momentum transfer region from 4 nm^{-1} to 27 nm^{-1}. The selected set of scans is presented in Fig. 1.

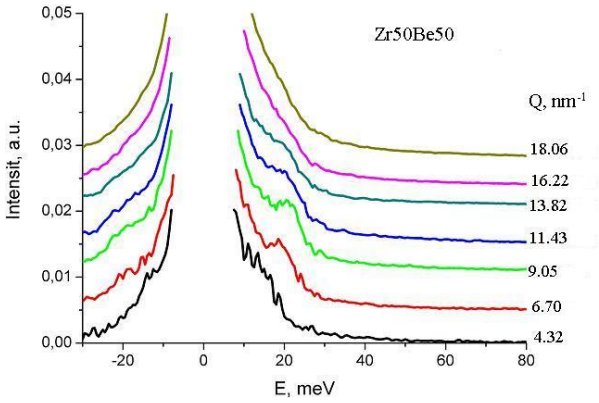

Fig. 1. IXS spectra of $Zr_{50}Be_{50}$ at the indicated fixed Q values.

Most reasonably the measured inelastic signal in region of 20 meV can be ascribed to an acostic propagating mode. An optical mode was supposed to appear at the energy range 40 - 60 meV. A commonly accepted procedure of data treatment is a spectra fitting by model DHO functions convoluted with the

resolution plus an elastic line. The instrumental response function has been recorded by measuring the scattering from a cooled (10K) disordered sample (Plexiglas).

It turned out that an elastic contribution, obtained by such methods, do not correspond well to the ZrBe spectra. A comparison of the BeZr spectrum and resolution function for analyzer 5 at different Q-setting is presented in Fig. 2.

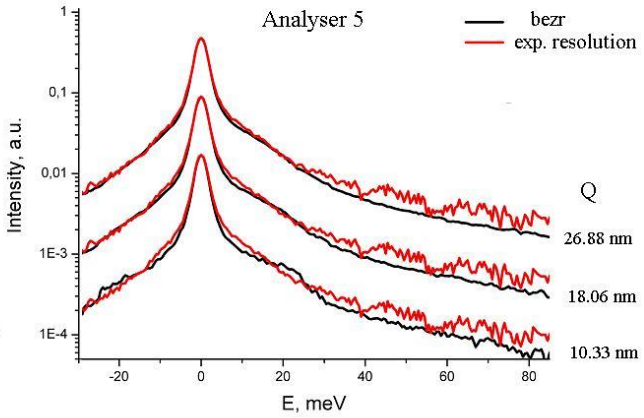

Fig. 2. The bezr sample response (black line) and experimental resolution (red line) of analyzer **5** for low (10.33 nm^{-1}), middle (18.06 nm^{-1}) and high (26.88 nm^{-1}) Q-settings.
The spectra are shifted upwards for clarity.

The resolution function exceeds the BeZr spectrum almost in the entire energy region. In this case extracting information about the acoustic and optic modes is not possible.

A comparison of the BeZr spectrum and resolution function for analyzer 3 at different Q-setting is presented in Fig. 3.

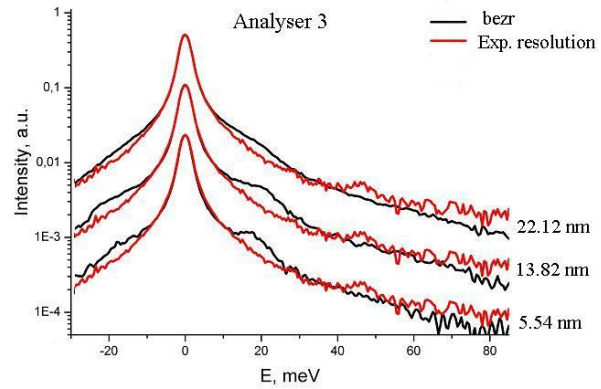

Fig. 3. The bezr sample response (black line) and experimental resolution (red line) of analyzer **3** for low (5.54 nm^{-1}), middle (13.82 nm^{-1}) and high (22.12 nm^{-1}) Q-settings.
The spectra are shifted upwards for clarity.

The resolution functions exceed the BeZr spectra at low energy region (up to 10 meV) and at high energy region (beyond 35 meV). In Fig. 4 the inelastic signals is depicted in form of current correlation function, $E^2/Q^2S(Q,E)$.

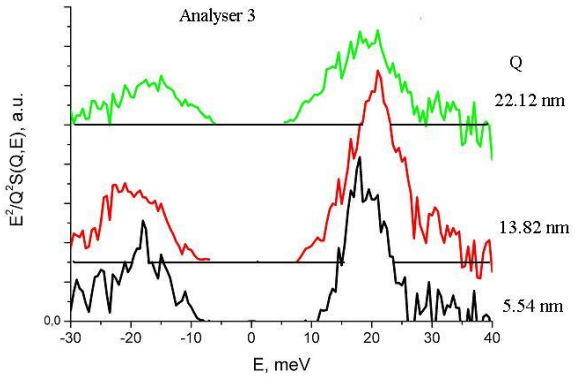

Fig. 4. The inelastic signal as measured by analyzer **3** for low (5.54 nm^{-1}), middle (13.82 nm^{-1}) and high (22.12 nm^{-1}) Q-settings. The spectra are shifted upwards for clarity.

Though the acoustic signal is clearly visible, a detailed analysis of the results fails because of absence of the low energy part of spectrum.

Some analyzers have shown much more reasonable picture. The resolution function of these analyzers becomes higher than the sample response only above 50 - 60 meV. A comparison of the BeZr spectrum and resolution function for analyzer 1 at different Q-setting is presented in Fig. 5. In Fig. 6 the inelastic signals for analyzers 1, 2 and 6 are depicted in form of longitudinal correlation function, $E^2/Q^2S(Q,E)$.

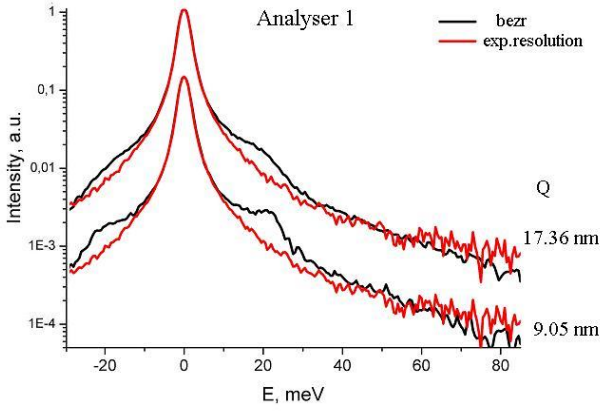

Figure 5. The bezr sample response (black line) and experimental resolution (red line) of analyzer **1** for middle (9.05 nm^{-1}) and high (17.36 nm^{-1}) Q-settings.

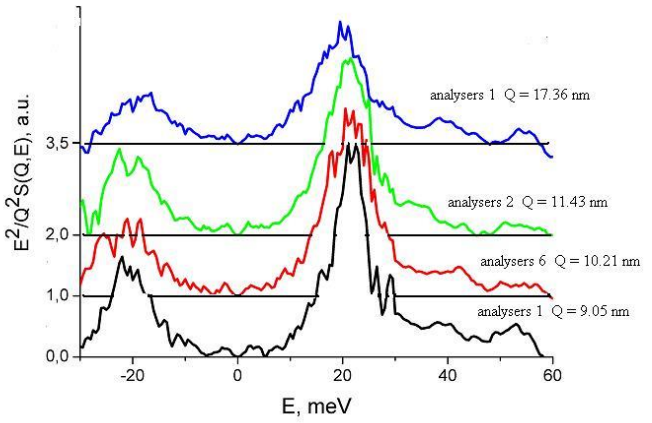

Figure 6. The inelastic signal as measured by analyzer **1, 6** and **2** for middle (9.05 nm^{-1}, 10.21 nm^{-1}, 11.43 nm^{-1}) and high (17.36 nm^{-1}) Q-settings.

Experimental data obtained with the analyzers 1,2, and 6 permit us to extract a peak position and width for acoustic-like mode. A presence of intensity above 30 meV indicates that optic-like mode may be registered. The difficulty of the search for optic mode lies in the fact that we are looking for a weak signal on a high wing of the Lorentzian resolution function. Therefore the high-frequency tail of the instrumental response function must be measured very accurately in order to yield reliable information on the elastic contribution. This issue we address to a folow-up proposal in which we intend to realise a self-consitent way of the instrumental response function determination. A measurement of ZrBe sample at low temperature (10K) will give us an exact instrumental response at a left-hand side of spectrum (anti-Stokes side). In this case there are no excitations present in the sample, so no scattering can occur with the annihilation of excitations. At a right-hand side of spectrum (Stokes side) the instrumental response will be admixed by the ZrBe sample response since excitations can be created by transfer of energy from the incident photon, of course. A measurement of ZrBe sample at high temperature (300 K) will give us an exact ZrBE sample response at a left-hand side of spectrum (anti-Stokes side). Using the detailed balance condition will help us to divide a right-hand side of spectrum (Stokes side) on two components – the ZrBe sample response and the instrumental response. Detailed balance remains valid when a single scattering creates or annihilates multiple excitations – a detailed balance between forward and reverse processes still exists because the thermodynamic probabilities of the required initial states are set by E. A practical use of detailed balance to check the quality of IXS experimental data is more convenient than of INS data because a required condition $\Delta Q(E) = \Delta Q(-E)$ is satisfied exactly. In the neutron experiment with time-of-flight chopper spectrometer this relationship is not symmetric. Also a noise background in IXS experiment usually is less than in INS one.

[1] G.F. Syrykh, et al. J. Phys.: Condens. Matter **20,** 104241 (2008).