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Report:

Abstract

The dynamic structure factor of a sodium silicate glass sample has been measured by inelastic X-rays scattering (IXS) as a function of the exchanged wave-vector Q at a fixed temperature $T = 600$ K, below its glass transition temperature ($T_g \sim 730$ K).

The sample was prepared with a 40% sodium concentration. The spectra in the low Q range ($1-5 \text{ nm}^{-1}$) are characterized by a peculiar negative dispersion of the longitudinal speed of sound followed by a positive dispersion.

Experiment and results

The dynamic structure factor has been measured for eight Q -sets of the five analyzer spectrometer arm. The Q -set were chosen so as to span with great detail (about 20 points in Q) the low wave-vector range $Q < 5 \text{ nm}^{-1}$, as apparent from panel B) of figure 1. An integration time of around 5 minutes/point, corresponding to a total time of 15 hours/spectrum, was used in order to achieve the very good signal to noise ratio that can be appreciated in panel A) of the figure.

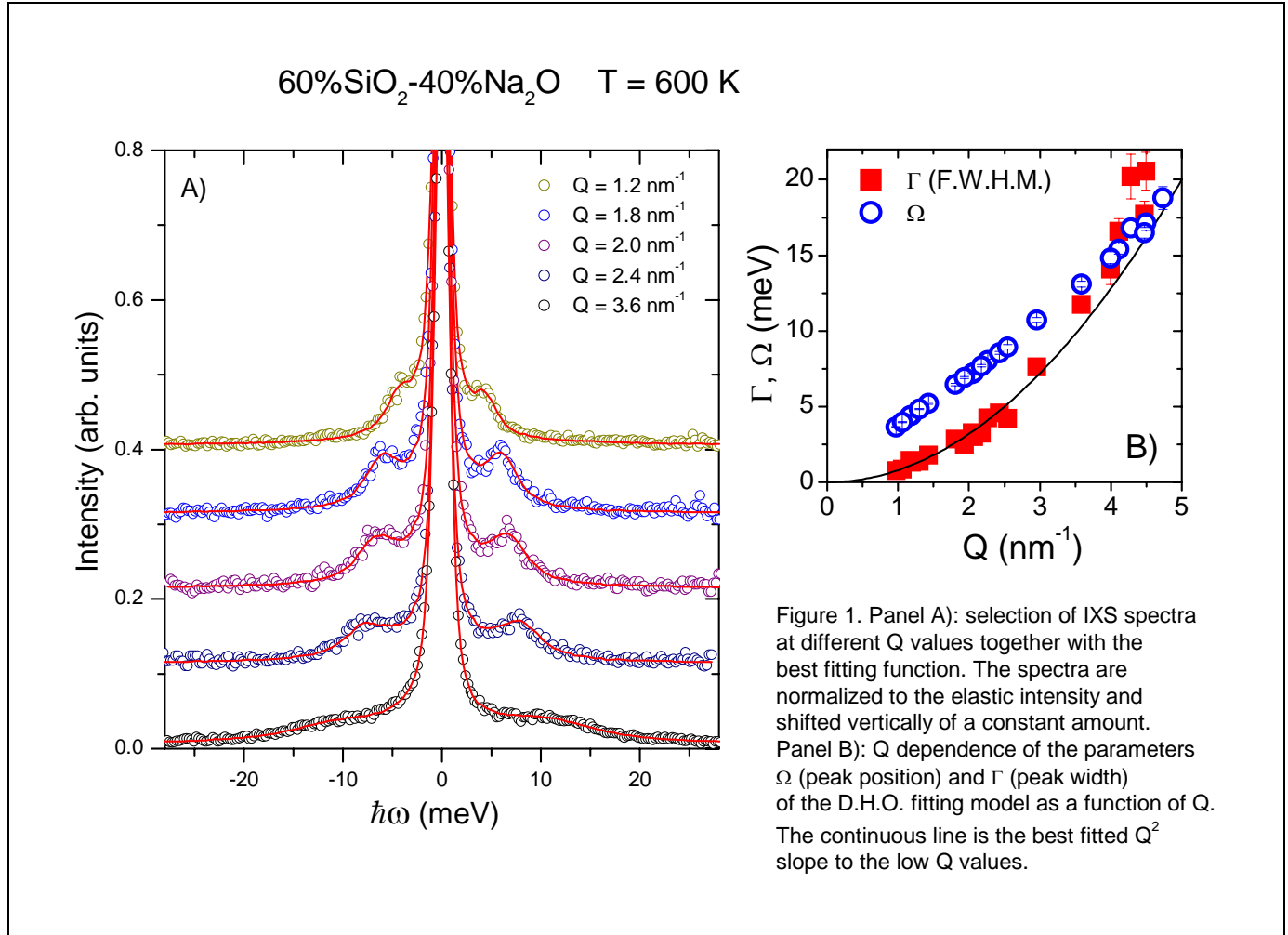
The spectra present a good elastic to inelastic intensity ratio, in agreement with the increased fragility characterizing this sample with respect to pure vitreous silica.

The spectra have been fitted to a damped harmonic oscillator (D.H.O.) function convoluted to the instrumental resolution plus an elastic line whose shape is given by the resolution itself. The apparent speed of sound, computed from the D.H.O. parameter Ω which describes the position of the inelastic peaks shows a peculiar negative dispersion between $Q = 1 \text{ nm}^{-1}$ and $Q = 2 \text{ nm}^{-1}$, followed by an increase at higher wave-vectors. To our knowledge the simultaneous presence of a negative and a positive sound velocity dispersion in a glass was never reported before.

The negative dispersion appears in a region where the peaks are well defined, with a width (the parameter Γ of the DHO function represents the F.W.H.M. of the peaks at low Q) which is still sensibly smaller than their

position Ω . On the contrary the positive dispersion appears when Γ approaches Ω . This happens for $Q \sim 4 \text{ nm}^{-1}$, as shown in panel B) of the figure.

It is worth noting that the negative dispersion appears at $Q \sim 2 \text{ nm}^{-1}$, which corresponds to an energy $\hbar\omega \sim 7 \text{ meV}$ (see panel B)), where the Boson Peak (BP) is expected from Raman data. To further investigate the connection between the excess of modes at the Boson Peak and the peculiar acoustic dispersion here observed a neutron time of flight experiment is scheduled in April at the IN6 spectrometer of the ILL.



Quite surprisingly the peculiar negative dispersion is not followed by any anomaly in the wave-vector dependence of the sound damping parameter Γ . This, in fact, follows a Q^2 behavior, whose nature is still unclear but is commonly associated to the broadening induced by the structural disorder.

In other glassy systems the parameter Γ shows a Q^4 behavior at Q values corresponding to energies below the BP position.

The change in slope of the damping at $Q = 2 \text{ nm}^{-1}$, the expected position of the BP and the Q value where the negative dispersion vanishes, between a Q^4 and a Q^2 laws may here be hidden by anharmonic contributions, since the experiment has been performed at $T = 600 \text{ K}$ in order to enhance the inelastic spectral features.

We have thus submitted a new proposal in order to investigate this possibility and to pursue the study of the dynamics in this class of materials. In particular it would be of much interest to measure a second sample with a lower sodium concentration in order to see whether the negative dispersion indeed follows the BP position, which should shift to lower energies when the sodium concentration is reduced, approaching the BP energy of pure ν -SiO₂, around 4 meV.