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|  | <b>Experiment title:</b><br>'Umklapp' processes in v-GeO <sub>2</sub>        | <b>Experiment number:</b><br>HS 1998 |
| <b>Beamline:</b><br>ID16   | <b>Date of experiment:</b><br>from: 16 November 2002<br>to: 24 November 2002 | <b>Date of report:</b><br>27/02/2003 |
| <b>Shifts:</b><br>21   | <b>Local contact(s): Dr Paola GIURA</b>                                      | <i>Received at ESRF:</i>             |
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### Report:

The problem of the dynamical properties of strong glasses in the mesoscopic range of energies and wavevectors, is one of the most debated issues in the physics of glassy materials. Glassy germania (v-GeO<sub>2</sub>) is a good candidate for this kind of investigation because: (i) its sound velocity is lower than that of v-SiO<sub>2</sub>, and (ii) in v-GeO<sub>2</sub> coherence effects are expected to be more effective than in silica. In spite of these potentially good properties, the first measurements performed on this material gave very poor signal, if any. So we decided to study another strong glass former, less promising in principle, i.e. vitreous Silica.

Accurate runs at constant exchanged wave-vector ( $Q^* = 6.5, 9.0, 11.5, 14.0, 16.5 \text{ nm}^{-1}$ ) were performed as a function of the energy E. This allowed us not only to measure the standard  $S(Q,E)$ , but also to have a sufficient signal-to-noise ratio in the high energy tails in order to obtain a reliable estimate of the current spectra  $C(E,Q^*) = E^2 * S(E,Q^*)$ . These spectra contain the relevant information about the dispersion relation, and should allow us to understand if in these glasses the excess in the density of states (usually referred to as Boson Peak) has a longitudinal or a transverse character, and possibly to evidence the presence in v-SiO<sub>2</sub> of the so called anomalous dispersion.

Computer simulation allows the dispersion curve of vitreous silica to be estimated and results in a plot as shown in figure 1. The maximum of the longitudinal currents (triangles), after a linear growth with a sound velocity of about 6000 m/s, shifts towards higher energies with increasing Q, with a steeper slope. This is a clear symptom of the presence of anomalous dispersion. On the contrary, the maximum of the transverse currents (squares) saturates at  $Q^*$  bigger than typically  $6 \text{ nm}^{-1}$ , and remains centred at about 15-20 meV irrespective of  $Q^*$ . In the figure, are also reported available Inelastic X-Ray Scattering experimental data in the low  $Q^*$  region (experiments HS 851 and HS 1307), as well as Inelastic Neutron Data (circles). According to the simulations, the spillover of the transverse dynamic in the longitudinal current spectra, would yield a

double peaked structure in the experimental currents in the  $Q$  range from about 5 to 10  $\text{nm}^{-1}$ . At higher  $Q^*$ 's, the longitudinal peak should displace with  $Q$ , while the low-energy one should remain constant. Diamonds in figure 1 indicate the position of the peaks observed in the current spectra in the present experiment.

In Figure 2 is shown the experimental current spectrum taken at  $Q^*=6.5 \text{ nm}^{-1}$  together with the computer simulation prediction. A double peaked structure is evident in both traces, even if the signal to noise ratio at the higher energies is still rather poor. In the spectra taken at higher  $Q^*$ 's this effect is less evident since the longitudinal peak shifts toward higher energies where the statistic is unfavourable.

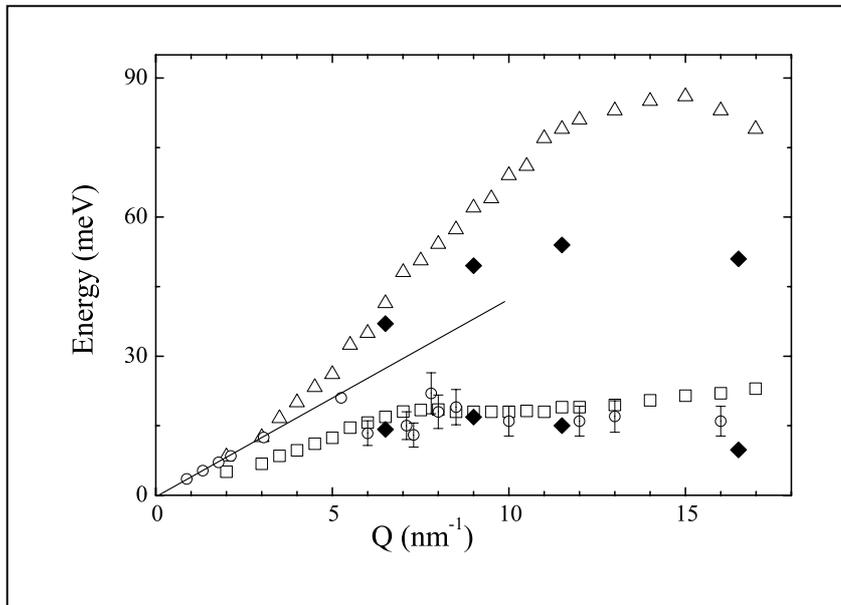


Figure 1.  
Dispersion curve for  $v\text{-SiO}_2$ . Triangles: maximum of computed longitudinal currents. Squares: maxima of computed transvers currents. Circles: previous experimental data (IXS and INS). Diamonds: this study.

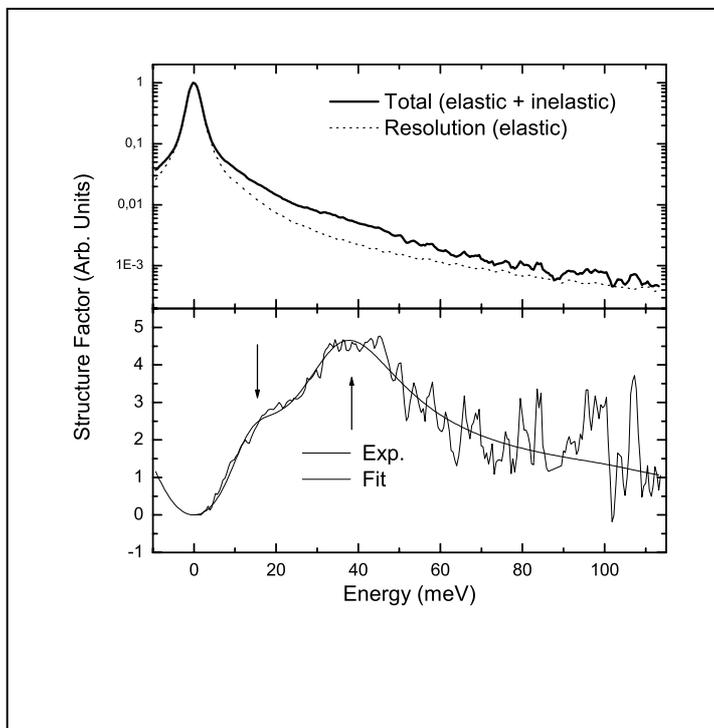


Figure 2.  
Top: Total (full line) and resolution (dotted line) IXS spectra at  $Q^*=6.5 \text{ nm}^{-1}$ . in a semilog scale. Bottom: inelastic contribution and relative fit, the two contributions peaking at about 15 and 35 meV are marked by arrows.