	Experiment title: High Q excitations in v-silica and silica xerogels	**Experiment number**: HS- 1307
Beamline: ID16	**Date of experiment**: from: 04-oct-00 7:00 to: 11-oct-00 7:00	**Date of report**: 25-feb-01
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Report:

The experiment HS-1307 was planned to confirm the existence and clarify the nature of "Umklapp"-like processes in disordered materials by studying the *Q*-dependence of excitations in the meV energy range around the first sharp maximum in the *S(Q)* of the vitreous silica. Only v-silica was studied to obtain a good statistic on the experimental data.

The experimental protocol used in this measurements of the Dynamic Structure Factor *S(Q,E)* consisted of *Q*- scans taken at constant energies (*E*) in the region ranging from below to well above the Boson Peak (BP) energy.

Our previouis results using this experimental protocol on the v-SiO_2 sample have shown well defined Brillouin peak in the low-*Q* region, well separated from the elastic contribution and a broad inelastic peak in the region of *Q* greater than about 15 nm^{-1} (Ref.[1]). On the contrary the IXS data reported previously for vitreous silica (v-SiO_2) taken varying *E* at Constant *Q* values, even at the highest investigated temperature, the inelastic contribution is observed as a weak shoulder on the tail of the elastic line due to the low value of the inelastic to elastic scattering ratio in v-SiO_2 as can be seen in Fig. 2 of Ref.[2].

Our measurements taken as constant *E* cuts (*E* ranging from 3.5 to 20 meV) as a function of *Q* present clearly a well defined Brillouin peak in the IXS spectra of amorphous silica superimposed to an almost *Q*-independent background due to elastic contribution, convoluted to the instrumental response function. The position and lineshape of the Brillouin peak has been deduced in all the energy scan, and it was found to follow the dispersion law up to the highest measure energy (20 meV).

We utilized the Si(11 11 11) configuration. The spectra at constant *E* and as a function of *Q* were made in two steps. In a first measurements, the spectra were taken in range from –2 to 32 nm^{-1} by using the five analyzers. The region below 6 $nm^{-1}$was studied in more detail and with a better accuracy using the analyzer number two with a *Q* resolution of 0.4 nm^{-1} fwhm. Two spectra taken at the constant energy of *E*= 3.5 and 20.0 meV are reported in Figure (open circles) . These two energies of observation were chosen to be below and well above the BP respectively, while the *E*=0 spectra (full lines in Figure) gives the *Q* dependence of the elastic background. This latter spectrum consists, in the measured *Q* range, only of an intense FSDP centered at about 15 nm^{-1}. Directly in the raw data of Figure one can see at low *Q* the existence of defined structures whose *Q* position changes almost linearly with *E* , while their widths increase with *E*. The presence of these peaks observed at a defined *Q* in the S(Q,E) in the constant energy guarantees the spatially non-localized nature of these excitations, and, in particular, of their propagating nature.

The FSDP is rather broad and structured showing in the high *Q* tail a shoulder centered at about 20 nm^{-1} where the contribution of Si-Si distance is expected. The observed inelastic contribution (dotted line in figure) is centered at energies higher than those of the FSDP is then ascribed to the first replica of the Brillouin peaks, due Umklapp processes. These are expected to lie near the wavevector corresponding to the Brillouin zone edge in the corresponding crystal at 16 nm^{-1}. Although this quantity cannot be defined in glasses is expected in v- SiO_2 at $Q > 16$ nm^{-1}. The inelastic structure becomes broader at higher energies evolving to an increasing tail. This suggests that even high *Q* vibration, belonging roughly speaking to the border of the Brillouin zone, maintain a defined *Q* vs *E* relationship.

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/2/P. Benassi, M. Krisch, C. Masciovecchio, V. Mazzacurati, G.Monaco, G. Ruocco, F. Sette, R. Verbeni, Phys. Rev. Lett. 77 (1996) 3835