



	Experiment title: High Q excitation in silica xerogels.	Experiment number: HS-851
Beamline: ID16/BL21	Date of experiment: from: 04-Feb-1999 to: 11-Feb-1999	Date of report: 24-Feb-2000
Shifts: 18	Local contact(s): Cunsolo Alessandro	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Maurizio Montagna, Aldo Fontana, Gabriele Viliani, Flavio Rossi, Oreste Pilla Dip. Fisica, Univ. Trento and INFN Povo I-38050, Italy. Maurizio Ferrari CEFSA-CNR 38050 Povo, Trento, Italy. A. Mermet, E.S.R.F BP 220, Grenoble, France. Giancarlo Ruocco, Dip. di Fisica, Universita' di L'Aquila, I-67100, L'Aquila, Italy.		

Report:

The aim of the experiment HS-851 was to assess the existence and 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 chosen system. The choice of different samples, each one corresponding to a different density and having a different width of its First Sharp Diffraction Peak (FSDP), is motivated by the aim to investigate whether it exists a relation between these excitations and the properties of the FSDP. 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 of the Boson Peak (BP). The first results on the reference sample of $v\text{-SiO}_2$ have shown unexpectedly well defined Brillouin peak in the low- Q region, well separated from the elastic contribution. In fact in the IXS data reported so far for vitreous silica ($v\text{-SiO}_2$), 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 $v\text{-SiO}_2$ as can be seen in Fig. 2 of Ref.[1]. These data have been utilized in different works both to claim the localized nature and to demonstrate the propagating nature of the collective excitations. In order to deduce from these data the existence of Brillouin peaks, as well as their positions, widths and lineshape to be compared with the theoretical predictions, a best fit and a deconvolution of the instrumental contribution are needed.

It is a matter of fact that these experimental data do not give a clear-cut indication allowing the choice of one of the contrasting models. Our measurements taken as constant E cuts as a function of Q present the *direct experimental evidence* of the existence of well defined Brillouin peaks in the IXS spectra of amorphous silica observed without any data manipulation. The elastic contribution, convoluted to the instrumental response function, shows up as an almost Q -independent background which does not affect significantly the position and lineshape of the Brillouin peak, so allowing its direct observation in the spectra. 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 the $-2 \div 32 \text{ nm}^{-1}$ range by using the five analyzers. The $-2 \div 6 \text{ nm}^{-1}$ region were studied in more details and with a better accuracy using the analyzer number two with a Q resolution of 0.4 nm^{-1} fwhm. The spectra taken at the constant energy of $E=5.3$ and 8.5 meV are reported in Figure (open circles). These two energies of observation were chosen to be on the maximum and on the high frequency tail of the Boson Peak 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 well defined structures peaking at 1.25 nm^{-1} in the $E=5.3 \text{ meV}$ cut and 2.1 nm^{-1} in the $E=8.5 \text{ meV}$ cut, whose Q position changes almost linearly with E , while their widths increase with E . The presence of peaks observed at a defined Q in the $S(Q, E)$ in the constant energy cuts is the fingerprint of the existence of a strict relationship between E and Q of the involved vibrational excitations i.e. of the spatially non-localized nature of these excitations, and, in particular, of their propagating nature. The observed effect was so relevant to settle the open question on the propagating or non-propagating nature of the high frequency modes in $v\text{-SiO}_2$ that we decided to use the total beam time for the measurements on vitreous silica and no time was left for the xerogel samples.

/1/P. Benassi, M. Krisch, C. Masciovecchio, V. Mazzacurati, G. Monaco, G. Ruocco, F. Sette, R. Verbeni, Phys. Rev. Lett. 77 (1996) 3835

