ESRF

Experiment title: Dependence of the boson peak of densified silica on the scattering vector	Experiment number: HS-1646

Beamline: ID28	Date of experiment: from: 09 Sep. 2001 to: 18 Sep. 2001	Date of report: October 4, 2002
Shifts: 24	Local contact(s): Dr. Alain Mermet	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
Pr. Marie FORET Laboratoire Des Verres, Université Montpellier II
Pr. Eric COURTENS ”
Dr. René VACHER ”
Dr. Benoit RUFFLÉ ”

Report:
In most glasses, a large number of vibrational modes, in excess to the Debye density of states, are found at frequencies near 1 THz. These modes produce a feature in the inelastic structure factor, the “boson” peak, which has been extensively studied by Raman and by inelastic neutron scattering. The nature of these modes is still a matter of debate. Another open question is the relation between the boson peak and the acoustic phonons of glasses. In the THz range, inelastic x-ray experiment show that these phonons are strongly broadened [1]. A likely interpretation is that plane-wave phonons cannot exist at frequencies above a Ioffe-regel crossover frequency of ~ 1 THz. It were very important to understand the possible relation between this crossover and the boson peak. A quite detailed measurement of the boson peak of silica with inelastic neutron scattering has been reported by Buchenau *et al.* [1]. Recent hyper-Raman scattering data revealed that both in normal and in densified silica the boson peak is associated with librations of the SiO_4 tetrahedra [2], which agrees with the earlier suggestion of Buchenau [1].
We investigated on ID28 the scattering vector dependence of the boson peak in densified silica, d-SiO_2, for Q ranging from 13.5 to 50 nm^{-1}. The measurements were performed at elevated temperature 565 K in order to increase the inelastic contribution to the spectra. At this T, the densified structure does not relax over the duration of the experiment. Fig. 1a, shows a typical raw spectrum obtained in 12 hours at $Q = 51$ nm^{-1}, after the usual monitor normalization. One clearly observes over the wings of the strong central elastic peak, shown as the dotted line, the broad inelastic contribution from the boson peak (BP).

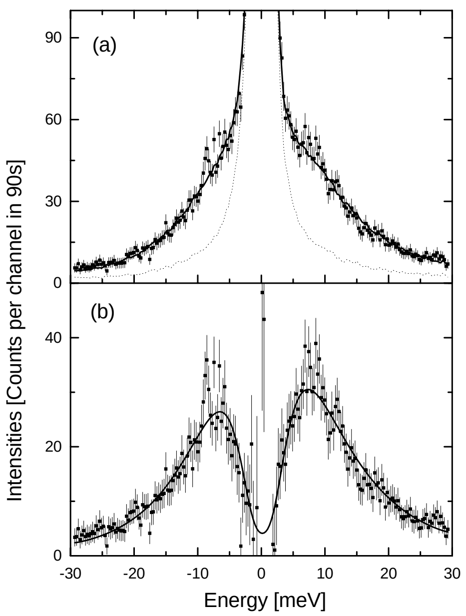

Figure 1

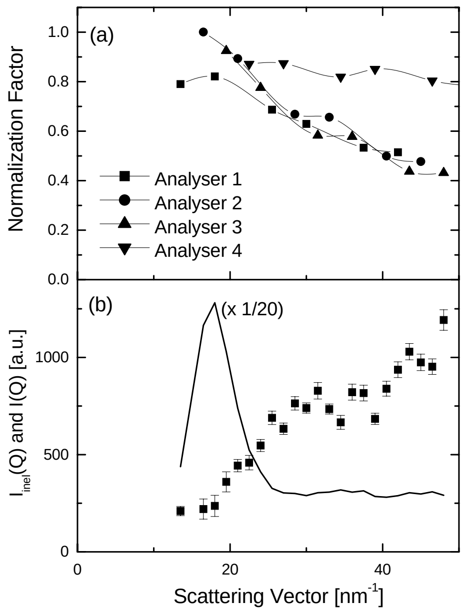

Figure 2

To extract information on the intensity and the position of the boson peak, the full spectra have been ajusted to a log-normale function plus an elastic central peak, convoluted with the instrumental function. A small background is added which is fixed to the electronic noise of the detectors. Fig. 1b illustrates the BP signal and its fit at $Q = 51$ nm^{-1}. Special care was taken to achieve a single relative scale for the intensities at all Q's. Indeed, the collected intensity could change with Q owing to a slight change in the focusing of the analysers onto the small collection holes placed 6 m away in front of the detectors. To correct for such an artefact the measured signal was scaled with a normalization factor obtained by comparing the integrated scattered signal to an independant measurement of the static structure factor of the sample at the same T. Fig. 2a shows the normalization factors deduced for the four available analysers. One should note that the correction is as strong as 100% at the highest investigated Q. Finally, Fig. 2b illustrates the evolution of both the strengh of the BP contribution and the total integrated intensity $I(Q)$. As already known from neutron measurements in normal v-SiO_2 [2], the main trend of the BP signal is to grow in Q^2, strongly modulated, however, by an inelastic structure factor $I^{(1)}(Q)$ different from $S(Q)$. The first sharp diffractation peak located at nearly 18 nm^{-1} is infact absent from $I^{(1)}(Q)$. That confirms the non acoustic nature of the boson peak modes already found in v-SiO_2 [2]. A quantitative analysis of $I^{(1)}(Q)$, including atomic form factor corrections and numerical simulations is under progress.

References

[1] M. Foret, R. Vacher, E. Courtens, G. Monaco, Phys. Rev. B **66** 024204 (2002).

[2] U. Buchenau, M. Prager, N. Nücker, A.J. Dianoux, N. Ahmad, W.A. Phillips, Phys. Rev. B **34** 5665 (1986).

[3] B. Hehlen, E. Courtens, R. Vacher, A. Yamanaka, M. Kataoka, K. Inoue, Phys. Rev. Lett. **84** 5355 (2000).