Dynamic Structure factor of 3-methylpentane

The dynamic and static structure factor of 3-methylpentane was measured in a wide range of temperature (from T=60K up to room temperature) and exchanged wave-vector (from 1 up to 12 nm^{-1}). The experimental data let to follow the evolution of the vibrational dynamics of the system in the transition from the liquid to the glassy phase which take place at T_g = 80 K.
A set of representative IXS spectra taken at different momentum transfers are reported in Fig. 1 and Fig.2 for T= 63K and 150K respectively. The Brillouin peak shift and broadens as the momentum transfer increases. In order to extract quantitative information on the q dependence of the parameters describing the peaks, the spectra were fitted by a model function made up by the convolution of the experimental resolution function with S(q,ν) represented by the sum of a δ-function and a damped harmonic oscillator for the elastic and inelastic contributions, respectively:

$$S(q,\nu) = \frac{S(q)}{2\pi^2}\left[f(q)\delta(\nu) + \left[1 - f(q)\right]\frac{\Omega^2(q)\Gamma(q)}{\left[\nu^2 - \Omega^2(q)\right]^2 + \nu^2\Gamma^2(q)}\right] \quad (1).$$

where the symbols have the usual meaning. The performed measurements cover the high frequency regime and contribute to completely characterize the vibrational dynamics of the system. As an exemplum, the temperature dependence of the sound velocity is reported in fig.3, for different exchanged wavevectors, from q=0.0038nm^{-1} measured at low frequency by transient grating technique (TG); the intermediate range probed by Brillouin light scattering in visible (BLS) and ultraviolet range (IUVS) with q=0.024 nm^{-1} and q=0.09nm^{-1} respectively; and finally the high frequency limit probed by inelastic X ray scattering (IXS) is also reported. The measure of the sound velocity from above the critical temperature (T_c ~ 100K), allow us to obtain a more reliable estimate of the so called infinite frequency sound velocity, c_∞, i.e. the velocity with all the relaxations blocked. We obtain the temperature dependence of c_∞ as shown in fig.3, that is a key ingredient in the analysis of relaxation processes and of great help in discerning between different generalized hydrodynamic models. The obtained results has to be submitted to international journals.

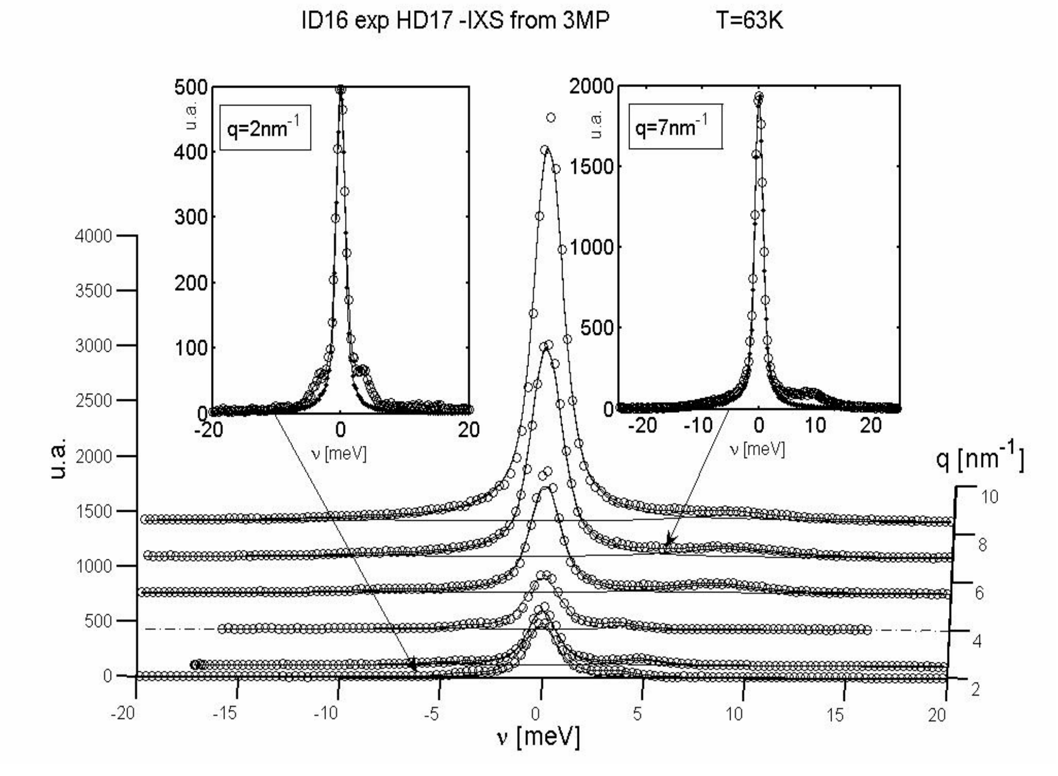

Figure 1: Experimental data (circles) and best fit using function (1) (lines) are reported for the investigated exchanged q at T=63K.

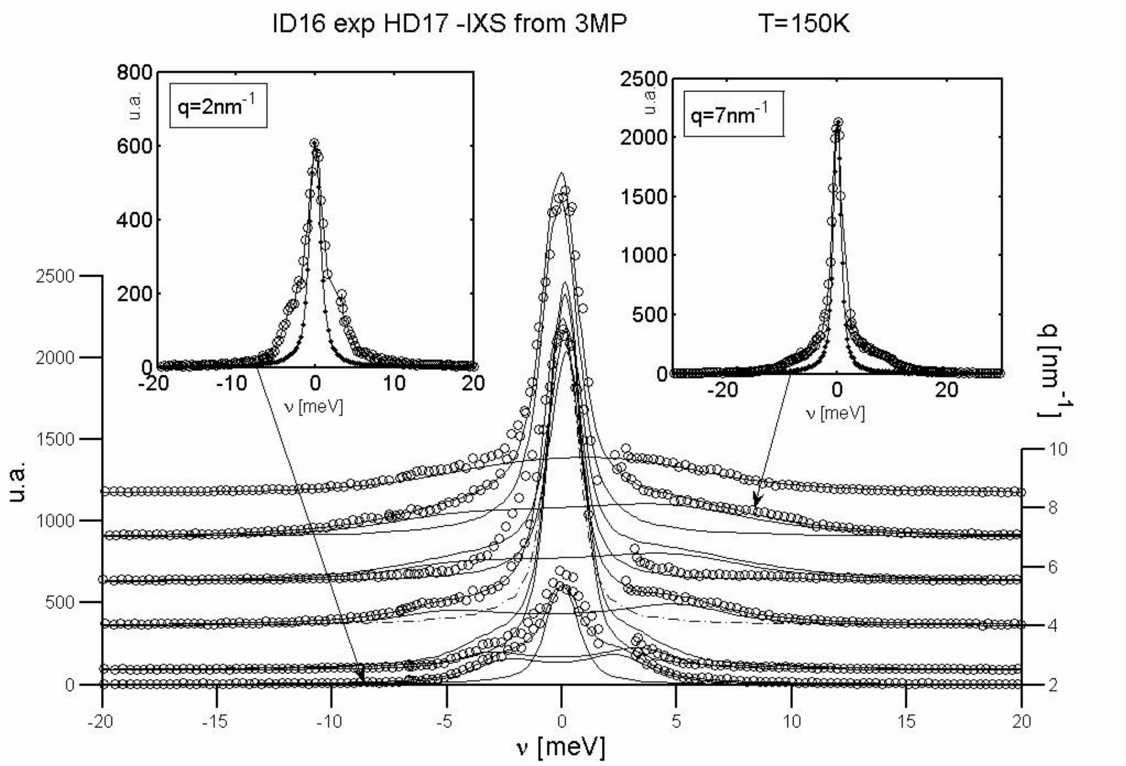

Figure 2 Experimental data (circles) and best fit using function (1) (lines) are reported for the investigated exchanged q at T=150K

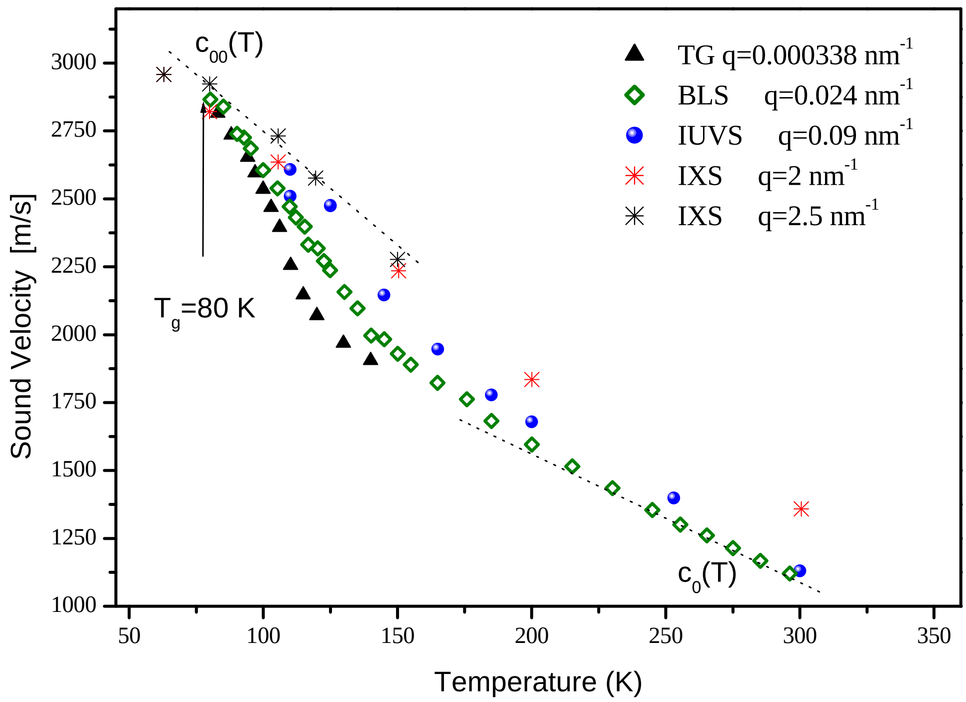

Figure 3: Temperature dependence of the hypersonic sound velocity at different frequencies.