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Report:

We studied energy spectra of collective motions in dibutyl phthalate (DBPh) glass with nuclear inelastic scattering [1] using ferrocene (Fc) and decamethyl ferrocene (DMFc) probe molecules. The probes contain a resonant Fe⁵⁷ nucleus at their center of mass. Measurements of nuclear inelastic scattering of x-rays by these nuclei allow one to determine the energy spectrum of probe motions driven by the glass matrix. According to our earlier studies [2], this approach selects collective vibrational motions of the glass and is not sensitive to local modes.

The aim of the experiment was an investigation of the universal dependence of vibrational density of states (DOS) in glasses. In previous studies [2], we found that at the energy region above the boson peak, the reduced DOS of *collective motions* exhibits precisely exponential behavior $g(E)/E^2 \propto \exp(-E/E_0)$. The characteristic energy of the exponential slope E_0 shows a correlation with the energy of the boson peak E_B . The task of this experiment was to check a possible dependence of the experimental data to the concentration of the probes and the size of the probe molecules.

Energy dependence of nuclear inelastic scattering was measured with an energy resolution of 0.5 meV. To study the concentration dependence, we performed a set of measurements at the same temperature of 22 K with the concentration of the Fc probes of 3 and 5%, and with the concentrations of the DMFc probes of 1% and 3%. For both probes, the derived DOS shows no concentration dependence.

On the other hand, we observed a difference in the data obtained with DMFc and Fc probes. The derived reduced density of states at 22 K is given below in linear and logarithmic scales. Short horizontal lines show the Debye approximation. In agreement with the previous results [2], the reduced DOS of collective motions measured with both probes (i) reveals an excess of vibrational modes (the boson peak) at low energy and (ii) shows a universal exponential dependence $g(E)/E^2 \propto \exp(-E/E_0)$ at high energy.

The data for two probes converge below the boson peak and increasingly diverge at higher energy. We attribute this trend to an effect of the probe size. The probes are sensitive to those collective vibrations, whose localization length is larger than the probe size. The volume of the DMFc probe is approximately two times bigger than that of the Fc probe (452 and 207 Å³, respectively). The characteristic localization length of atomic vibrations is known to decrease with their energy. Accordingly, the larger DMFc probes show progressively lower number of states at higher energy.

In our previous studies [2], we observed a correlation between the energy position of the boson peak E_B and the exponent E_0 . The present data confirm this trend: The DMFc data show a boson peak at lower energy and an exponential slope with faster decay (smaller E_0).

In conclusion, the obtained experimental results confirm the existence of a universal law for DOS in glasses at the energies above the boson peak. In addition, they reveal the dependence of the measured DOS on the probe size. Using a set of probe molecules with significantly different sizes, this dependence can be utilized to study the localization length of atomic vibrations in glasses.



References:

1. see, e.g., A. Chumakov and W. Sturhahn, Hyp. Interact. 123/124 (1999) 781.

2. A. Chumakov et al, submitted to Phys. Rev. Letters, see also experimental report HS1931.