

2024

Nanostructures and Applied Spectroscopy research group:

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Topology of nanoclusters and the characteristic of Boson peak in As-S glasses. — The combination of mean coordination and concentration dependencies of elastic modules and low-frequency Raman scattering of As-S glasses brings new information about the spectroscopic Boson peak (SBP) behavior (Fig. 1a, b). The analysis of the characteristic temperature positions of the thermometric Boson peak (TBP) and the magnitude of heat capacity of As-S glasses was performed (Fig 2). This study was focused on the As-S compounds from the first glass-forming region with particular attention to the compositions of flexible, intermediate, and stressed-rigid phases. The origin of SBP and TBP is expected to have a structural nature. The spectral features found in the super low-frequency region of Raman spectra were assigned to quasi-localized "soft" modes.

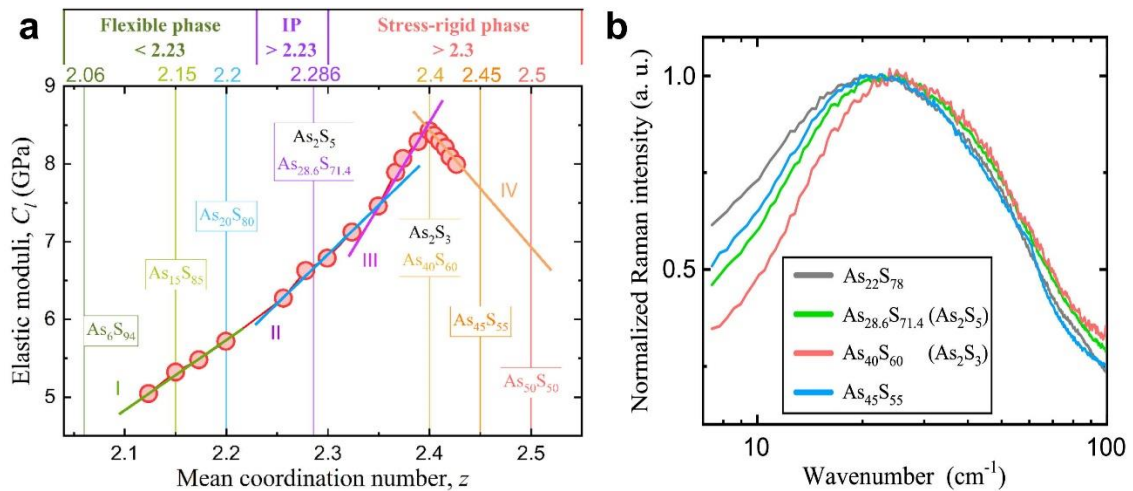


Figure 1. (a) Mean coordination number (z) dependence of longitudinal elastic moduli C_l ; **(b)** Reduced and normalized SBP of As_xS_{100-x} glasses.

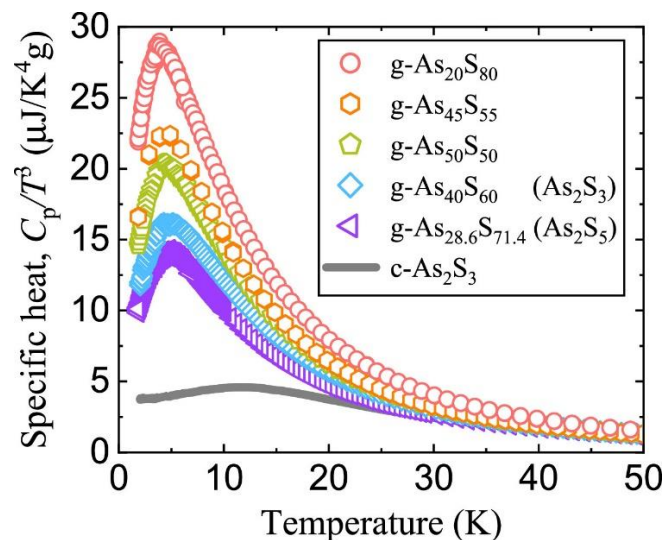


Figure 2. Temperature dependence of the reduced specific heat C_p/T^3 for various As-S samples.

The sulfur-rich glass, g-As₂S₅, represents the intermediate phase with As_nS_m clusters containing closed ends and several "soft" nanoclusters. These soft clusters can be responsible for intrinsic quasi-localized "soft" modes, the overall rigidity of the system, and quasi-elastic light scattering.

It was shown that the change in intensity and position of TBP and SBP is associated with the evolution of composition in four elastic regions of glasses. The correlation between the compositional dependence of SBP and TBP was established, demonstrating interconnection with elastic and other properties of As-S glasses. Experimental evidence of a slight growth of specific heat intensity for the stress-rigid composition with $z = 2.4$ compared to the composition from the intermediate region with $z = 2.28$ ($x = 28.6\%$) was found. The U-shape compositional dependence of the TBP position is assumed to correlate with the contribution of localized vibration modes within the large (medium-range order scale) "soft" nanoclusters and long branchy clusters' vibrations. The nanocluster types with prevailing As-As or S-S bonds and their concentrations, influencing the SPB and TBP positions, strongly depend on the ratio between As and S atoms. The intensity of the super low-frequency ($<20 \text{ cm}^{-1}$) light scattering spectrum has the same U-shape dependence on connectivity, similar to the TBP dependence on composition.

References:

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