Tata Institute of Fundamental Research

Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Students' Annual Webinar

Enhanced Vibrational Stability in Open Boundary Amorphous Solids

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In contrast to crystals whose vibrational states are well described by the Debye model of solids, amorphous solids exhibit anomalous mechanical and thermal properties. Amorphous solids possess an excess of low-frequency modes over and above the Debye prediction. It has been suggested that the large specific heats of glasses and the plastic failure of amorphous solids originate due to these low-frequency non-phononic vibrational modes. Numerical studies of recent times have identified that VDoS of amorphous solids follow a universal quartic scaling in the low-frequency regime. However, in some studies, deviations from universal quartic law are reported. In this talk, I will discuss some of these previous studies along with our new findings for amorphous solids prepared in open boundary conditions. We show that in amorphous solids prepared in open boundary conditions, there are significantly fewer low-frequency vibrational modes when compared to their periodic boundary counterparts. Specifically, we find that the universal $D(\omega) \sim \omega^4$ law changes to $D(\omega) \sim \omega^\delta$ with $\delta \approx 5$ in two dimensions and $\delta \approx 4.5$ in three dimensions. Crucially, this enhanced stability is achieved under slow annealing protocols whereas fast quenches reproduce the ω^4 behaviour. We perform an anharmonic analysis of the minima corresponding to the lowest-frequency modes in such open-boundary systems and discuss their correlation with the density of states. A study of various system sizes further reveals that small systems display a higher degree of localisation in vibrations. Lastly, we confine open-boundary solids in order to introduce macroscopic stresses in the system which are absent in the unconfined system, and find that the $D(\omega) \sim \omega^4$ behaviour is recovered.

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4:00 PM (Tea / Coffee 3.45 PM)

Seminar Hall, TIFR-H