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The ω^3 scaling of the vibrational density of states in quasi-2D nanoconfined solids

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Atomic vibrations play a vital role in the functions of various physical, chemical, and biological materials. The vibrational properties and the specific heat of a bulk material are well described by the Debye theory, which successfully predicts the quadratic w^2 low-frequency scaling of the vibrational density of states (VDOS) in bulk solids from few fundamental assumptions. However, the corresponding relationships for nanoconfined materials with fewer degrees of freedom, have been far less well explored. The effects of confinement on the VDOS of glasses and amorphous solids have been discussed in several works with particular attention to the fate of the Boson Peak anomaly and glassy relaxation dynamics. Few discussions have been made on the scaling of VDOS of other solids under confinement or its foundations. Learning how GOM modifies the vibrational dynamics of glass formers, is of utmost significance to understand and optimize the phonon-assisted transportation of energy, electron or proton in various electronic devices and biological systems of nano-meter confinement.

In this work, inelastic neutron scattering was used as an experimental method to investigate the VDOS of ice in the sandwich of graphene oxide thin film at different confined sizes. We found that the low frequency scale of the dynamic vibration density of ice in the sandwich changed from w^2 in Debye's model to w^3 at a faster rate as the confined size decreased. All atomic molecular dynamics (MD) simulations confirm the experimental results and show that the scale changes are equally applicable to crystal and amorphous ice.

We developed a simple geometric model, deducing that this power comes from the phase space constraints imposed by the unidirectional confinement of the solid. Based on the model, we predicted that the Debye scale would be at a particular frequency. The quantitative prediction was reappeared and validated by MD simulations

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