The Boson Peak in Crystals; A Remembrance of Things Past

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ABSTRACT In recent years, in thermal, optical, and neutron measurements of phonons, at $T/\Theta_D \sim 10^{-3} - 10^{-2}$, a large excess density of states over the Debye prediction is widely observed. This apparent anomaly has become known as the Boson Peak (BP). Many recent observations have been made in non-crystalline materials, where in a much lower temperature range ($T/\Theta_D \sim 10^{-4}$), special tunneling states due to the disorder cause linear temperature dependence of specific heat, but this is not our concern here. It has also then been assumed that the BP, in itself, is a signature of the disordered (glassy) states. However, going back into the literature of the past 50 years, one finds a) Boson peaks are equally found in very good crystals, b) Historically the failure of the Debye approximation at temperatures $T/\Theta_D > 10^{-3}$ was often noted and analyzed, just where the BP is observed. This gives us pause.

DISCUSSION Going further, historically, various measurements in the '60s and '70s made on materials which could be prepared in both crystalline and amorphous forms (we discuss Ge in detail) showed BP that were, within a few percent, identical to each other (with adjustment for density)! Clearly, just on experimental grounds BP was not a signature of disorder. The distinguishing feature of Ge and other diamond structure elements is the importance of directed bonds. We discuss physically from straight-forward heuristic models of such materials (conventional thermodynamic harmonic correlation functions) how the BP can arise generally, and can have intrinsic spatially localized vibrational character (i.e. embryos) in the harmonic regime, in either crystalline or amorphous materials. We conclude that a) The BP is not a signature of glassy structure per se, but a consequence of the nature of the bonding, b) Comparison with the Debye density of states as a base line is generally <u>unjustified</u>, anyhow, in the BP region. We discuss the origin of the apparently large BP in SiO2 glass as an artifact only.