When does a crystal conduct heat like a glass?

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Motivated by the search for improved thermoelectric materials, several compounds have attracted attention that combine the high electron mobilities found in crystals with a low thermal conductivity κ, approaching κ-values typical for glasses. The common structural feature of these "electron crystal phonon glass" (ECPG) materials is that they contain loosely bound atoms that reside in a large crystalline "cage". These "rattlers" scatter phonons and greatly reduce the thermal conductivity of the material, but generally not to quite glasslike levels. A particular class of clathrates is formed by the filled skutterudite antimonides [1]. More recently, the Ge-clathrate $Sr_8Ga_{16}Ge_{30}$ was found to be an ECPG material, having a truly glasslike thermal conductivity while maintaining the crystalline electronic properties [2, 3].
Here we report a combination of Resonant Ultrasound Spectroscopy, neutron-scattering, low-temperature ultrasonic attenuation and thermal conductivity measurements for filled and unfilled skutterudites and for Ge-clathrates. Taken together, these measurements suggest specific structural features that result in a crystal with the lowest possible thermal conductivity, namely that of a glass with the same chemical composition. The weakly bound atoms that "rattle" within the oversized atomic cages in the crystal result in a low thermal conductivity, but the present data show that both "rattling" *and* tunneling states are necessary to produce a true glass-like thermal conductivity.

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[2] J.L. Cohn et al., Phys. Rev. Lett. 82, 778-782 (1999).
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