Low thermal conductivity materials investigated using inelastic neutron scattering

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Reducing thermal conductivity without relying on unstable nanostructures and rare, environmentally unfriendly elements is a great challenge. The intermetallic clathrates - like $Ba_8Ga_{16}Ge_{30}$ - are a well studied family of material that fulfil this criterion. Clathrates are framework structures containing loosely bonded guest atoms. The guest atom has low energy phonon branches, which interacts with the heat carrying phonons, through an 'avoided crossing' between the guest atom mode and the acoustic branches of the host structure. The avoided crossing leads to a lowering of the phonon speed which in turn lowers the thermal conductivity. [1]

The type I tin clathrates, $A_8Sn_{44}[]_2$, A=Rb,Cs has been investigated using powder inelastic neutron scattering (INS). The phonon spectrum was measured at a range of temperatures to investigate anharmonic effects and the effect of the phase.

The investigation of tin clathrate reveal low energy phonon modes, not observed for Ge and Si clathrates. Owing to anharmonic effects and comparison to theoretical calculations [2] these modes are interpreted as the transverse acoustic branches of the host structure reaching the zone boundary without interacting with the guest mode, in opposition to Si and Ge clathrates.

1. Christensen, M., et al., Nature Materials, 2008. **7**(10): p. 811-815.
2. Tse, J.S., Z. Li, and K. Uehara, Europhysics Letters, 2001. **56**(2): p. 261-267.