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Heat conduction in thermoelectric materials

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Energy efficiency of existing sources can be improved by reducing heat losses, thermoelectric materials has the capability of interconverting between electricity and a temperature gradient. The wanted properties of thermoelectrics can be summarized, as the a "Phonon-Glass, Electron-Crystal"(PGEC) [1]. In host-guest systems, the host structure is considered to be the electron crystal, while low frequency guest atom modes reduces the acoustic phonons realize the phonon-glass part. The type-I clathrates are state-of-the-art host-guest material with respectable thermoelectric properties [2]. The structure consists of a Ga/Ge framework forming two dodecahedral and six larger tetrakaidecahedral cages, which are occupied by the guest guest atoms. The thermal conductivity of the clathrates are about 1 W/mK, which is the same order of magnitude as amorphous glass. Neutrons scattering has been used to elucidate structural and dynamic details in the clathrate system. Single crystal diffraction has been used to investigate the guest atom position in the large dodecahedral cage of Sr8Ga16Ge30 synthesized using three different methods. Triple axis spectroscopy has been used to investigate the phonon dispersion relation for Ba8Ga16Ge30. . The dispersion relation measured along (330)+[hh0] revealed avoided crossing between the acoustic phonons and the guest atom mode. To further investigate the phonon lifetimes Spin-echo triple axis spectroscopy measurements were carried out at TRISP at FRM-II.
The neutron scattering experiments have delivered valuable insight into the atomic structure and motion of the host-guest clathrates. The neutron scattering experiments show that the low thermal conductivity can attributed to low phonon group velocities, caused by the band flattening due to interactions between the host structure and the guest atom.[3] Through the results we have been able to explain the low thermal conductivity and the results offer guidance in the search for new materials with improved thermoelectric properties.

[1] G. A. Slack, CRC Handbook of Thermoelectrics, 407 (1995).

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