Systematic Studies on Anharmonicity of Rattling Phonons in Type I Clathrates by Low Temperature Heat Capacity Measurements

KATSUMI TANIGAKI, JIAZHEN WU, YOICHI TANABE, SATOSHI HEGURI, HIDEKAZU SHIIMOTANI, Tohoku Univ, TOHOKU UNIVERSITY COLLABORATION — Clathrates are featured by cage-like polyhedral hosts mainly composed of the IVth group elements of Si, Ge, or Sn and alkali metal or alkaline-earth metal elements can be accommodated inside as a guest atom. One of the most intriguing issues in clathrates is their outstanding high thermoelectric performances thanks to the low thermal conductivity. Being irrespective of good electric conductivity $\sigma$, the guest atom motions provide a low-energy lying less-dispersive phonons and can greatly suppress thermal conductivity $\kappa$. This makes clathrates close to the concept of “phonon glass electron crystal: PGEC” and useful in thermoelectric materials from the viewpoint of the figure of merit. In the present study, we show that the local phonon anharmonicity indicated by the tunneling-term of the endohedral atoms ($\alpha T$) and the itinerant-electron term ($\gamma_e T$), both of which show T-linear dependences in specific heat $C_p$, can successfully be separated by employing single crystals with various carrier concentrations in a wide range of temperature experiments. The factors affecting on the phonon anharmonicity as well as the strength of electron-phonon interactions will be discussed based on our recent experiments.

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