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Systematic Studies on Anharmonicity of Rattling Phonons in Type I Clathrates by Low Temperature Heat Capacity Measurements[1]
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 σ, the guest atom motions provide a low-energy lying less-dispersive phonons and can greatly suppress thermal conductivity κ. 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 (αT) and the itinerant-electron term (γ_eT), 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 temperture experimennts. 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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