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Examining Lattice Disorder in Type-I Clathrate $Ba_8Ga_{16}Sn_{30}$ using EXAFS[1] SCOTT MEDLING, MICHAEL KOZINA, FRANK BRIDGES, UC Santa Cruz, KOICHIRO SUEKUNI, Japan Advanced Institute of Science and Technology, TOSHIRO TAKABATAKE, Hiroshima University — Semiconducting type I clathrates, such as $Ba_8Ga_{16}Ge_{30}$ (BaGaGe) and $Ba_8Ga_{16}Sn_{30}$ (BaGaSn), have a cage-like crystal structure with "rattler" atoms (Ba) located near the center of cages (Ga-Ge/Sn). Such compounds have a low thermal conductivity which is attributed mainly to vibrations of the "rattler" atoms inside the cages which strongly scatter phonons. BaGaSn has a surprising lower thermal conductivity than BaGaGe. To better understand why, we studied samples of BaGaSn using Extended X-ray Absorption Fine Structure (EXAFS). The analysis shows that the average Ga-Sn distance is shorter and the average Sn-Sn distance is longer than the distances found from diffraction; also, the Ba-Ga and Ba-Sn distances have greatly increased disorder. This suggests that the cage-like structure is severely distorted, in contrast to BaGaGe; such a large distortion will strongly scatter phonons, decreasing the thermal conductivity, but unfortunately also will reduce the electrical conductivity. We compare our results for BaGaSn with earlier results for BaGaGe and discuss them in light of recent transport measurements.

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