研究論文

層状酸化カルコゲン化物 LaCuSeO の高密度多結晶における熱電変換性能の一軸加圧異方性

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Anisotropic Thermoelectric Exchange Properties of High Density Polycrystalline Layered Oxychalcogenide, LaCuSeO obtained by Uniaxial Hot Pressing

by

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(Received Jan. 17, 2018; Accepted Jan. 25, 2018)

Abstract

Undoped LaCuSeO is an electrically insulating mixed anion layered compound (MALC) with an optical band gap Eg ~2.7 eV. Anisotropic thermoelectric exchange properties of uniaxially hot-pressed (HP) polycrystalline LaCuSeO, which is a representative MALC with ZrCuSiAs-type structures, are demonstrated. We defined directions for the measurements parallel/vertical to the pressing axis as $P_{//}$ / $P_{\perp}$. A crystallographic anisotropy of the polycrystalline LaCuSeO is verified by a ratio between Bragg diffraction intensities with Miller indices 003 and 110 in a tetragonal lattice. XRD patterns of $P_{//}$ and $P_{\perp}$ show weakly *a*-axis and *c*-axis oriented crystallographic phases. While undoped LaCuSeO shows a high resistivity with $\rho = 1.0 \times 10^2$ Ωm and does not show measureable Seebeck coefficient at room temperature, ρ of the $P_{//}$ and $P_{\perp}$ show ~60 times smaller than that of undoped. $P_{//}$ and $P_{\perp}$ exhibit a finite large Seebeck coefficient (*S*) with ~800 μVK^{-1} at $T \sim 400$ K . The smaller ρ are mainly due to a hole doping by slight crystallographic defects induced via hot-pressing process.

Keywords: Layered oxychalcogenide, LaCuSeO, Hot press, Transport properties, Seebeck effect

1. 緒言

熱電変換は導体の両端に温度差を与えると，起電力が生じる Seebeck 効果[1]を利用して，温度差から電力を生み出す技術である．熱電変換の最大変換効率(Carnot 効率)は導体の輸送特性，すなわち電気抵抗率 ρ，熱伝導率 κ，Seebeck 係数 S，および絶対温度 T を用いて，Ioffe により(1)式[2]で定義された無次元性能指数(ZT)にて律される．

$$ZT = \frac{S^2}{\rho\kappa} T \quad (1)$$

高い熱電変換性能を示す純物質は現在まで盛んに探索された．しかしながら，室温付近における最大の ZT は 1954 年に Goldsmid らにより報告された Bi_2Te_3[3]の $ZT = 0.77$ が最高であり，Bi_2Te_3 を超える新規な熱電変換材料の出現はエネルギーハーベスティング技術の発達に必要である．

ZrCuSiAs 型[4]の層状アニオン化合物(Mixed Anion Layerd Compounds， MALC)は，透明 p 型半導体 LaCuSO[5]，

平成 30 年 1 月 17 日受付

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