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Crystal structure and thermoelectric properties of kuramite $Cu_3Sn(Se,S)_4$ with cation disorder YOSUKE GOTO, YOICHI KAMIHARA, MASANORI MATOBA, Keio Univ, KEIO UNIV TEAM — Ternary or quaternary compounds Cu_2–T_M–A–Ch_4 (T_M; transition metal, A; group 14 or 15 elements, Ch; chalcogen) are promising p–type thermoelectric materials because of their heavy but still conducting valence band, which is composed of Cu $3d$ and Ch $3p$ orbitals. Lattice thermal conductivity should be suppressed by cation disorder, however, coexistence of transition metals such as Cu and Zn on quaternary compounds complicate the understanding of the details of cation disorder by means of conventional X-ray diffraction. In this work, We demonstrate the crystal structure and thermoelectric properties of kuramite $Cu_3Sn(Se,S)_4$. Structural analysis revealed that polycrystalline samples crystallize in tetragonal I–$42m$ space group. The $2a$ site was occupied by Cu only, while $2b$ and $4d$ sites were occupied by Cu and Sn partial disorder. Both electrical conductivity (σ) and Seebeck coefficient (S) were increased with substitution of Se for S, resulting $\sigma = 5.68 \times 10^2$ Scm^{-1} and $S = 114$ μVK^{-1} at 623 K, respectively. At the conference, we will also report the alloy effect on thermal conductivity of $Cu_3Sn(Se,S)_4$ solid solution.

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