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Thermoelectric properties and crystal structures in Y doped Ca₃Co₄O₉

H. Nakatsugawa , H. M. Jeong and K. Nagasawa

Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan

E-mail : naka@ynu.ac.jp

Thermoelectric oxides have been attracting increasing attention from the viewpoint of application to thermoelectric power generation using waste heat, because the candidate oxides are composed of environmentally benign elements and are chemically stable at a high temperature in air atmosphere. [Ca₂CoO₃]_{0.62}CoO₂, known as Ca₃Co₄O₉, have attracted much attention as candidate for p-type thermoelectric materials.[1] We studyed Y substitution effects on Ca site because an ion radius of Y^{3+} are close to that of Ca^{2+} . Polycrystalline samples of $[(Ca_{1,x}Y_x)_2CoO_3]_{0.62}CoO_2$ (0.00 $\leq x \leq 0.05$) were synthesized by a conventional solid state reaction method. Starting powders of dried CaCO₃ (99.9%), Y₂O₃ (99.99%), Co₃O₄ (99.9%) were ground and heated at 1193K for 24h in O2. The crystallographic structure was analyzed with x-ray and neutron diffraction measurements. The neutron diffraction was carried out at room temperature using HERMES installed on T1-3 port of JRR-3M reactor in JAERI. The lattice parameters were refined using Rietveld analysis by PREMOS in the REMOS95 package. The magnetic susceptibilities were measured using a SQUID magnetometer (quantum design MPMS) as function of temperature on both field and zerofield cooling. We investigated the Y substitution effect on the thermoelectric and magnetic properties. With the Y substitution, both the electrical resistivity and Seebeck coefficient do not change drastically. This is attributed to the carrier concentration of samples. Seebeck and Hall coefficient measurements reveal that the major charge carriers in the samples are holes.

[1] H.Nakatsugwa, H.M.Jeong, R.H.Kim and N.Gomi, Jpn. J. Appl. Phys., in press.