High-temperature resistivity and thermoelectric properties of coupled substituted $Ca_3Co_2O_6$

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Abstract. Polycrystalline samples of $Ca_{3-x}Na_xCo_{2-x}Mn_xO_6$ (x=0.0–0.5) have been prepared by the sol-gel cum combustion method using sucrose in order to investigate the effects of the coupled substitution of Na and Mn on Ca and Co sites on the transport properties of $Ca_3Co_2O_6$(Co326). The products were characterized by Fourier transform infrared spectroscopy, powder x-ray diffraction (XRD), thermogravimetry (TGA), differential thermal analysis and scanning electron microscopy. XRD patterns reveal the formation of single-phase products up to x=0.5. Coupled substitution increases the solubility of both Na and Mn on Ca and Co sites, respectively, in contrast to the limited solubility of Na and Mn (x=0.2) when separately substituted. TGA confirms the formation of the $Ca_3Co_2O_6$ phase at temperatures ~720 °C. The grain size of the parent and substituted products is in the range 150–250 nm. Electrical resistivity and Seebeck coefficient were measured in the temperature range 300–800 K. Resistivity shows semiconducting behavior for all the compositions, particularly in the low-temperature regime. The Seebeck coefficient increases with temperature throughout the measured temperature range for all compositions. The maximum Seebeck coefficient (200 μV K^{-1}) is observed for x=0.5 at 825 K, and this composition may be optimal for high-temperature thermoelectric applications.

Keywords: Seebeck coefficient, resistivity, x-ray diffraction, sol-gel

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