Structure and thermoelectric properties of Ca$_{2-x}$Sr$_x$FeMoO$_6$ (0 $\leq$ x $\leq$ 0.3) double-perovskite oxides

The thermoelectric properties of double perovskite-type oxides Ca$_2$FeMoO$_6$ are investigated in terms of Sr substitution at the A site of the oxides. The electrical conductivity, $\sigma$, of Ca$_{2-x}$Sr$_x$FeMoO$_6$ (0 $\leq$ x $\leq$ 0.3) showed a metallic behavior, decreasing monotonically from ca. 103 S cm$^{-1}$ at room temperature to ca. 102 S cm$^{-1}$ at 1250 K. At room temperature, although the values of the oxides increased with increasing substitution level, x, the values maintained almost the same values at high temperature range of 1000–1250 K. The absolute values of the Seebeck coefficient, $S$, for the samples at x $<$ 0.3 abruptly increase at around 1000 K. The Rietveld refinement of the XRD patterns of the oxides indicated that the anti-site defects in the oxides decreased with increasing Sr concentration. The power factor, $S^2$, of the oxides largely increased with increasing temperature; the $S^2$ value of Ca$_2$FeMoO$_6$ was ca. 0.35 mW mK$^{-2}$ at 1200 K, the largest value of all the samples in this study. Although the thermal conductivity, $\kappa$, of the oxides generally decreased from ca. 3.5 to 4.5 W mK$^{-1}$ at room temperature to ca. 2–3 W mK$^{-1}$ at 1050 K, the sample at x = 0.3 showed the lowest and most T-independent values, implying that the relative increase in the temperature is independent from the phonon-impurity scattering caused by the A-site substitution. The power factor of the oxides increased above 900 K; thereby, the dimensionless figure of merit, $ZT = (S^2/\kappa)T$, significantly increased at the same temperature range. The largest ZT value of 0.15 was observed for Ca$_2$FeMoO$_6$, Ca$_{1.9}$Sr$_{0.1}$FeMoO$_6$, and Ca$_{1.8}$Sr$_{0.2}$FeMoO$_6$ at 1250 K. © 2012 Elsevier B.V. All rights reserved.

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