Journal of ELECTRONIC MATERIALS, Vol. 42, No. 7, 2013
DOI: 10.1007/s11664-012-2451-5

Thermoelectric Properties of $RuSb_2Te$ Ternary Skutterudites

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Polycrystalline samples of the $RuSb_2Te$ ternary skutterudite compound were prepared by the powder metallurgy method, and the influence of various types of doping on its thermoelectric properties was studied. The phase purity of the prepared samples was checked by means of powder x-ray diffraction, and their compositions were checked by electron probe x-ray microanalysis. Hot-pressed *p*-type samples were characterized by measurements of electrical conductivity, Hall coefficient, Seebeck coefficient, and thermal conductivity. Various doping strategies, i.e., cation substitution ($Ru_{0.95}Fe_{0.05}Sb_2Te$), anion substitution ($RuSb_2Sn_{0.1}Te_{0.9}$) or partial filling of voids of the ternary skutterudite structure ($Yb_{0.05}RuSb_2Te$), were investigated, and the influence of the dopants on the changes of the resulting transport, thermoelectric, and thermal properties is described.

Key words: $RuSb_2Te$, ternary skutterudite, doping, thermoelectric properties, thermal conductivity, thermoelectric figure of merit

INTRODUCTION

Almost two decades after skutterudite compounds were identified as prime candidate novel thermoelectrics,[1,2] these materials have been proved viable for thermoelectric applications. Due to the presence of large voids in their crystal structure, skutterudites seem to be good candidates for fulfilling the phonon-glass electron-crystal (PGEC) concept[2] of superior thermoelectric materials. These empty voids, which can be filled with various atoms, are believed to produce important phonon scattering, resulting in a significant reduction in lattice thermal conductivity κ_L and consequently superior thermoelectric properties.[3,4] Intense research on improving the thermoelectric properties of skutterudites has led to preparation of skutterudite-based materials that consistently attain improved ZT values either by multiple filling[5,6] or by preparation of thermoelectric nanocomposites.[7,8]

Ternary skutterudites are a special category of compounds derived from binary skutterudites (with general formula MX_3, where M = Co, Ir or Rh; X = P, As or Sb). In contrast to their binary counterparts, these materials offer various possibilities for improving the thermoelectric performance, e.g., lowering the lattice thermal conductivity or considerable change of bandgap values.[9] Ternary skutterudites can be obtained either by isoelectronic substitution on the cation site M by a pair of elements from group 8 and 10, e.g., $Fe_{0.5}Ni_{0.5}Sb_3$,[10] or by analogical substitution on the anion site X by a pair of elements from group 14 and 16 of the Periodic Table, e.g., $CoGe_{1.5}Te_{1.5}$,[11] or alternatively by simultaneous substitution on both cation and anion sites, e.g., $FeSb_2Te$.[9]

The existence of the ternary skutterudite $RuSb_2Te$ was mentioned in Fleurial's list[9] of prospective ternary skutterudites, but comprehensive thermoelectric study of this compound including doping is still lacking. In our recent publication[12] we reported the structural refinement of the compound using the Rietveld method. According to that work, the phase displays cubic symmetry (space group $Im\ \overline{3}$), and no structural ordering of Sb and Te atoms was observed. The aim of this article is to present a study of the influence of various types of substitution on both

(Received July 4, 2012; accepted December 28, 2012; published online February 20, 2013)