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Thermoelectric properties of bulk β-Indium sulfide with Mg doping

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Abstract

An *ab initio* calculation indicated that the low temperature phase of indium sulfide, β-In_2S_3 has a potential to be good thermoelectric materials. The thermoelectric properties of Mg-doped β-In_2S_3 above room temperature were investigated at the first time.

The bulk samples of $In_{2-x}Mg_xS_3$ (x =0, 0.05, 0.1, 0.2 and 0.3) were prepared by pulsed current sintering using the powder obtained from the solid reaction of raw elements in a sealed silica tube. All bulk samples showed high relative density over than 90%. The powder X-ray diffraction (XRD) patterns of all samples were well indexed as β-In_2S_3 structure without any second phases. The peaks shift to the lower diffraction angles indicating the increasing of lattice parameter of magnesium-substituted samples. This result sounds strange because ionic radius of magnesium is smaller than indium, and presumably indicates the simultaneous formation of vacancies on magnesium-substitution.

The thermoelectric properties of Seebeck coefficient (S), electrical resistivity (ρ), and thermal conductivity (κ) were measured at temperature range from 300 K to 700 K. The maximum power factor (S^2/ρ) for non-doped In_2S_3 is 426.5 μW/mK^2, which was slightly higher than that of magnesium substituted samples at the same temperature. On the other hand, the thermal conductivity κ at 300 K significantly decreased from 1.64W/mK for the non-doped sample to 1.10 W/mK for the sample with x = 0.2. (Fig.1) The reduction in κ may attribute to the increasing of point defect scatting caused by the anharmonic oscillation of atoms in the vicinity of vacancies. The maximum dimensionless figure of merit $ZT = S^2T/\rho\kappa$ for non-doped In_2S_3 and magnesium doped sample (x = 0.1) were 0.38 and 0.45 at 700 K, respectively.

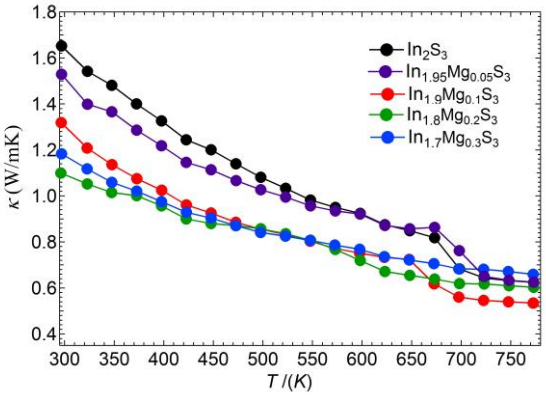

Fig. 1 Temperature dependence of thermal conductivity observed for $In_{2-x}Mg_xS_3$ (x = 0, 0.05, 0.1, 0.2 and 0.3).