Ag で部分置換した Mg_2Sn の結晶構造と熱電特性

The Crystal Structures and Thermoelectric Properties of Ag-doped Mg_2Sn

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Thermoelectric (TE) materials, which can directly convert waste heat into electricity, are expected to play a significant role in future energy utilization. The performance of TE materials is evaluated in terms of the dimensionless figure of merit, $zT = S^2\sigma T/\kappa$, and power factor $PF = S^2\sigma$, where S, σ, T, and κ are the Seebeck coefficient, electrical conductivity, absolute temperature, and thermal conductivity, respectively. Mg_2Sn is a promising mid-temperature TE material consisting of earth-abundant, low cost, and less-toxic elements. Recently, we successfully prepared Mg_2Sn single-crystal ingots with Mg vacancy (V_{Mg}) by melting method under Ar pressure [1]. The V_{Mg} has an effect of lowing lattice thermal conductivity (κ_{lat}) of Mg_2Sn, which is lower than those of the Mg_2Sn polycrystals ever reported. Furthermore, we prepared n-type $Mg_2Sn_{1-x}Sb$ (x = 0.005, 0.01, and 0.02) single crystal ingots and investigated the effect of point defects and Sb doping on their crystal structures and TE properties [2]. Due to the higher carrier mobility and lower lattice thermal conductivity than those of the $Mg_2Sn_{1-x}Sb_x$ polycrystals, the maximum zT value of 0.72 at 650 K was achieved for the $Mg_2Sn_{0.99}Sb_{0.01}$ single crystal ingot.

As for p-type Mg_2Sn, we prepared $Mg_2Sn_{1-x}Ga_x$ single crystal ingots and investigated their TE properties. Although we obtained relatively low κ_{lat} for $Mg_2Sn_{0.98}Ga_{0.02}$ ingots, the zT value (zT_{max} = 0.17@450 K) were still now high enough because of the low carrier concentration (5.92×10^{19} cm^{-3}) [3]. In this work, Ag-doped Mg_2Sn ingots with V_{Mg} were prepared by the melting method, whose morphology and TE properties were investigated with a particular emphasis on effects of doped Ag atoms and V_{Mg}. The maximum PF (PF_{max} = 1.5 $mW\cdot m^{-1}\cdot K^{-2}$) was achieved for $Mg_{1.99}Ag_{0.01}Sn$ at 300 K, and the PF decreased with the temperature increased. This may be due to the influences of the secondary phase in the $Mg_{1.99}Ag_{0.01}Sn$ ingots. We will try to prepare $Mg_{2(1-x)}Ag_{2x}Sn$ single crystal by controlling the cooling rate during preparation, and investigate their V_{Mg} fraction, carrier concentration, and TE properties, which will be reported in the presentation.

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[1] W. Saito et al., *Sci. Rep.* 10 (2020) 2020.

[2] W. Saito et al., *ACS Appl. Mater.* (2020) DOI: 10.1021/acsami. 0c17462.

[3] Z. C. Huang et al., *ACT&SACT2020* AO0027.