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Thermoelectric properties of materials near the band crossing line in Mg₂Sn–Mg₂Ge–Mg₂Si system

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ABSTRACT

Thermoelectric properties of materials with compositions on and near the band crossing line connecting Mg₂Sn_{0.765}Ge_{0.22}Sb_{0.015} and Mg₂Sn_{0.685}Si_{0.3}Sb_{0.015} in the Mg₂Sn–Mg₂Ge–Mg₂Si system are investigated. Although ZTs are very similar, power factors are different. On the line, the power factor decreases from Mg₂Sn_{0.765}Ge_{0.22}Sb_{0.015} to Mg₂Sn_{0.685}Si_{0.3}Sb_{0.015}, and off the line, the power factor also decreases. The output power and energy conversion efficiency are calculated using engineering power factor (PF)_{eng} and figure of merit (ZT)_{eng}. It is shown that although similar energy conversion efficiency of ~11% could be achieved for all compositions studied, the output power are different, increasing from ~9.1 W cm^{−2} for Mg₂Sn_{0.685}Si_{0.3}Sb_{0.015} to ~10.3 W cm^{−2} for Mg₂Sn_{0.765}Ge_{0.22}Sb_{0.015}, due to the different power factors.

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1. Introduction

Thermoelectric materials, converting heat energy into electricity, have received extensive attentions due to their potential roles in increasing energy conversion efficiency in vehicles, boilers, solar generators, etc. [1–5]. Thermoelectric performance of power generation devices requires not only high conversion efficiency but also large output power [6,7]. On the basis of constant property model, the maximum energy conversion efficiency (η_{max}) and output power (ω_{max}) are related to material parameters figure of merit (ZT) and power factor (PF), respectively, as following [7].

$$\eta_{max} = \frac{T_H - T_C}{T_H} \left(\frac{\sqrt{1 + Z\bar{T}} - 1}{\sqrt{1 + Z\bar{T}} + T_C/T_H} \right) \quad (1)$$

$$\omega_{max} = \frac{1}{4} \frac{(T_H - T_C)^2}{L_{leg}} PF \quad (2)$$

where $Z\bar{T} = S^2\bar{T}/\rho\kappa$, $PF = S^2/\rho$, and $\bar{T} = (T_H + T_C)/2$, S is Seebeck coefficient, ρ is electrical resistivity, κ is thermal conductivity, L_{leg} is length of leg, T_H is hot side temperature, and T_C is cold side temperature.

For the Mg₂Sn–Mg₂Ge–Mg₂Si system, most of the research has focused on Mg₂Sn–Mg₂Si [8–23], with limited reports on Mg₂Sn–Mg₂Ge [7,24] and Mg₂Ge–Mg₂Si [25–29]. Improved ZT from Si alloying effects were early demonstrated in Mg₂Sn–Mg₂Si system, and the best property was achieved in Mg₂Sn_{0.6}Si_{0.4} [9]. Recently, there are increasing interests in reinvestigating the Mg₂Sn–Mg₂Si system around the composition of Mg₂Sn_{0.6}Si_{0.4} [10,11,16,19,22,23]. One of the investigations found that Mg₂Sn_{0.7}Si_{0.3} has higher power factor (~47 μ W cm^{−1} K^{−2} at 523 K) and hence higher ZT (~1.3 at 700 K) than Mg₂Sn_{0.6}Si_{0.4} due to the composition caused band crossing (or band convergence) [16]. Recently, Liu et al. reported Mg₂Sn_{0.75}Ge_{0.25} is even better than Mg₂Sn_{0.7}Si_{0.3} with higher PF (~55 μ W cm^{−1} K^{−2} at 623 K) and higher ZT (~1.4 at 723 K) with a similar band crossing in

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Mg₂Sn–Mg₂Ge system happened near the composition of Mg₂Sn_{0.75}Ge_{0.25} [7]. According to our recent understanding [30], in the Sn-poor region (purple in Fig. 1a), it would have a light conduction band (C_L -band) at the bottom which is mainly from the hybridized 3p orbital of Mg with the s-orbital and d- e_g orbital of IV elements (i.e., Sn, Ge, Si) as shown in Fig. 1b. In contrast, in the Sn-rich region (blue in Fig. 1a), it has a heavy conduction band (C_H -band) at the bottom which is the hybridization between 3s-orbital of Mg with the d- t_{2g} orbital of IV elements, shown in Fig. 1d. Thus, at certain composition, the C_L -band and C_H -band would converge, shown in Fig. 1c.

For Mg₂Sn_{0.75}Si_{0.3} and Mg₂Sn_{0.75}Ge_{0.25}, their high thermoelectric performance are mainly attributed to the band crossing. It is expected that the band crossing would also occur in compositions on and near the line connecting Mg₂Sn_{0.75}Si_{0.3} and Mg₂Sn_{0.75}Ge_{0.25} in the Mg₂Sn–Mg₂Ge–Mg₂Si system with a possibility of even higher thermoelectric performance. It is noted that there are several reports on thermoelectric properties of Mg₂Sn–Mg₂Ge–Mg₂Si system [23,24,31–33], as shown in Fig. 1a. Most of them are about partial substitution of Sn by Ge in Mg₂Sn_{0.6}Si_{0.4}, such as Mg₂Sn_{0.55}Ge_{0.05}Si_{0.4} and Mg₂Sn_{0.5}Ge_{0.10}Si_{0.4} [6]. However, from the band crossing map (Fig. 1b–d), substitution of Ge for Sn in Mg₂Sn_{0.6-y}Ge_ySi_{0.4} brings the material away from the line connecting Mg₂Sn_{0.75}Ge_{0.25} and Mg₂Sn_{0.75}Si_{0.3}, which lose the benefits of the unique band structure. Tada et al. [24] has conducted an investigation on Mg₂Sn_xGe_{0.1}Si_{0.9-x} ($x = 0.6, 0.65, 0.75, 0.9$), near the line. However, they only did the composition Mg₂Sn_{0.6}Ge_{0.1}Si_{0.3}, showing an n-type behavior and also poor electrical conductivity. To our best knowledge, there is still lack of investigation about the compositions on and near the line connecting Mg₂Sn_{0.75}Ge_{0.25} and

Mg₂Sn_{0.75}Si_{0.3} in the Mg₂Sn–Mg₂Ge–Mg₂Si system.

Therefore, the motivation of this work is to investigate the thermoelectric properties of materials in the Mg₂Sn–Mg₂Ge–Mg₂Si system on and near the line connecting Mg₂Sn_{0.78}Ge_{0.22} and Mg₂Sn_{0.75}Si_{0.3}. It is noted that Mg₂Sn_{0.75}Ge_{0.25} is slightly deviate from the theoretically predicted band crossing point of Mg₂Sn_{0.78}Ge_{0.22} [10]. In our previous work, Mg₂Sn_{0.75}Ge_{0.25} was investigated, while Mg₂Sn_{0.78}Ge_{0.22} has not yet been studied. In this work, we have studied compositions on and near the line connecting Mg₂Sn_{0.78}Ge_{0.22} and Mg₂Sn_{0.75}Si_{0.3}. The thermoelectric performances were further evaluated by using engineering power factor (PF)_{eng} and figure of merit (ZT)_{eng} [34], which consider the temperature dependence of thermoelectric properties over the whole temperature range of the hot and cold sides.

2. Experimental section

2.1. Synthesis

High purity magnesium turnings (Mg, 99.98%; Alfa Aesar), tin powder (Sn, 99.8%; Alfa Aesar), germanium powder (Ge, 99.9999%; Alfa Aesar), silicon shots (Si, 99.999%; Alfa Aesar), antimony shots (Sb, 99.999%; Alfa Aesar) were weighed according to the composition of Mg₂(Sn_{0.765}Ge_{0.22}Sb_{0.015})_{1-x}(Sn_{0.685}Si_{0.3}Sb_{0.015})_x ($x = 0, 0.2, 0.4, 0.6, 0.8, 1$). Moreover, samples near the line connecting Mg₂Sn_{0.765}Ge_{0.22}Sb_{0.015} and Mg₂Sn_{0.685}Si_{0.3}Sb_{0.015} were also prepared, i.e., Mg₂Sn_{0.685}Ge_{0.25}Si_{0.05}Sb_{0.015}, Mg₂Sn_{0.685}Ge_{0.15}Si_{0.15}Sb_{0.015}, Mg₂Sn_{0.735}Ge_{0.15}Si_{0.1}Sb_{0.015}, Mg₂Sn_{0.735}Ge_{0.05}Si_{0.2}Sb_{0.015}. For all the samples, 3 at% extra Mg were added in order to compensate the loss of Mg during the preparation. The elements were loaded into stainless

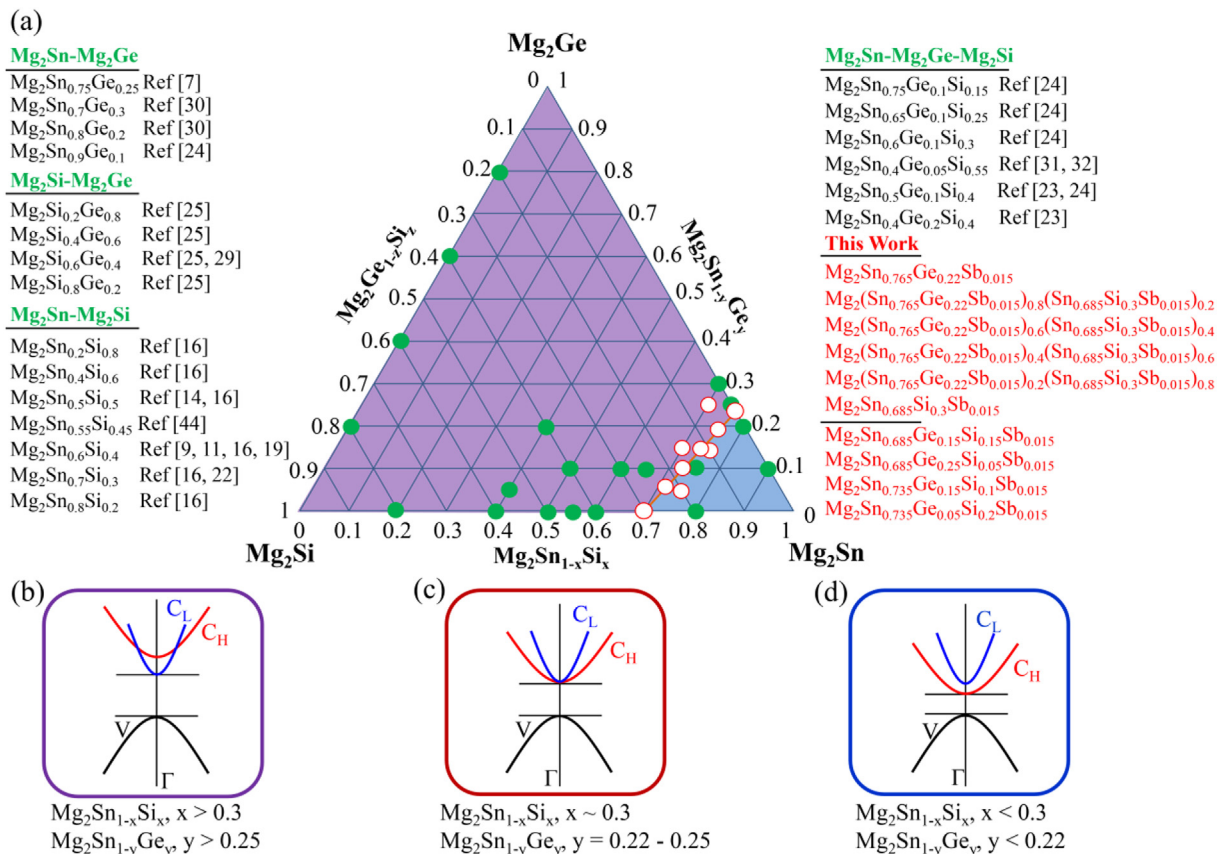


Fig. 1. (a) Research on the thermoelectric properties of materials in the Mg₂Sn–Mg₂Ge–Mg₂Si system, (b), (c) and (d) effects of composition on band convergence of Mg₂Sn–Mg₂Ge–Mg₂Si.

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