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Supplementary Information

Thermoelectric properties of Bi-based Zintl compounds $Ca_{1-x}Yb_xMg_2Bi_2$

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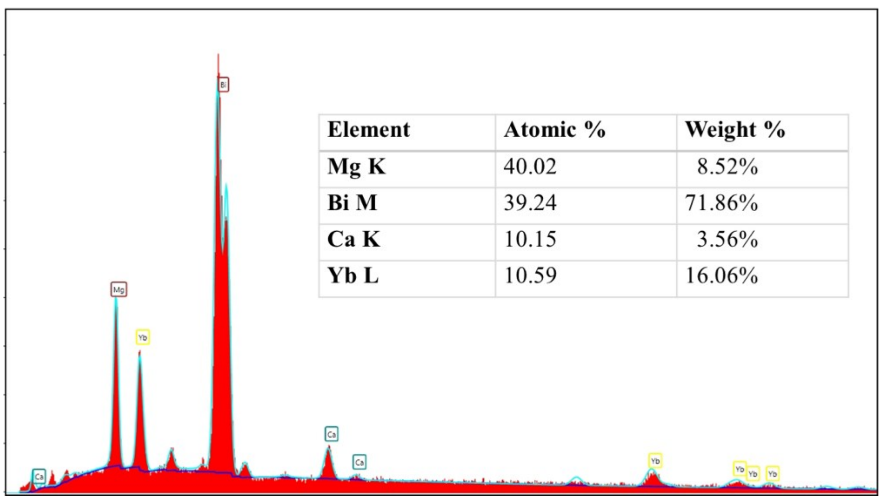

Element	Atomic %	Weight %
Mg K	40.02	8.52%
Bi M	39.24	71.86%
Ca K	10.15	3.56%
Yb L	10.59	16.06%

Fig. S1. EDS pattern of $Ca_{0.5}Yb_{0.5}Mg_2Bi_2$.

Calculated $(ZT)_{eng}$,$(PF)_{eng}$, output power density and leg efficiency

Kim *et al*. proposed the engineering dimensionless figure of merit $(ZT)_{eng}$ as a function of thermal boundaries, *i.e*., the temperatures of hot side T_h and cold side T_c, which is defined as,[1]

$$(ZT)_{eng} = \frac{\left(\int_{T_c}^{T_h} S(T)\,dT\right)^2}{\int_{T_c}^{T_h} \rho(T)\,dT \int_{T_c}^{T_h} \kappa(T)\,dT}(T_h - T_c) = \frac{(PF)_{eng}}{\int_{T_c}^{T_h} \kappa(T)\,dT}(T_h - T_c) \quad (1)$$

where $S(T)$, $\rho(T)$, and $\kappa(T)$ are temperature dependent thermoelectric properties, and $(PF)_{eng}$ is the engineering power factor with respect to the boundary temperatures. $(ZT)_{eng}$ implies the cumulative effect of TE properties at a given thermal boundary. $(PF)_{eng}$ has unit of W m^{-1} K^{-1}, different from the conventional unit of W m^{-1} K^{-2} due to its cumulative effect associated with the temperature gradient.

Assuming T_c = 323 K and 2 mm of leg length, we have calculated the maximum efficiency η_{max} and its corresponding output power density P_d including Thomson heat based on $(ZT)_{eng}$ and $(PF)_{eng}$ using the following formula.[1]

$$\eta_{\max} = \eta_c \frac{\sqrt{1+(ZT)_{eng}\alpha_1\eta_c^{-1}} - 1}{\alpha_0\sqrt{1+(ZT)_{eng}\alpha_1\eta_c^{-1}} + \alpha_2} \quad (2)$$

$$P_d = \frac{(PF)_{eng}\Delta T}{L} \frac{\sqrt{1+(ZT)_{eng}\alpha_1\eta_c^{-1}}}{\left(\sqrt{1+(ZT)_{eng}\alpha_1\eta_c^{-1}} + 1\right)^2} \quad (3)$$

where,

$$\alpha_i = \frac{S(T_h)\Delta T}{\int_{T_c}^{T_h} S(T)\,dT} - \frac{\int_{T_c}^{T_h} \tau(T)\,dT}{\int_{T_c}^{T_h} S(T)\,dT} W_T\eta_c - iW_J\eta_c \quad (i = 0, 1 \text{ and } 2) \quad (4)$$

$$W_J = \frac{\int_{T_c}^{T_h}\int_{T}^{T_h} \rho(T)\,dT\,dT}{\Delta T \int_{T_c}^{T_h} \rho(T)\,dT} \text{ and } W_T = \frac{\int_{T_c}^{T_h}\int_{T}^{T_h} \tau(T)\,dT\,dT}{\Delta T \int_{T_c}^{T_h} \tau(T)\,dT} \quad (5)$$

η_c is Carnot efficiency, and W_J and W_T are weight factors representing a practical contribution of Joule and Thomson heat affecting the heat flux at the hot side, respectively, based on their cumulative effect.

Reference:

1. H. S. Kim, W. S. Liu, G. Chen, C. W. Chu and Z. F. Ren, *Proc. Natl. Acad. Sci. U. S. A.,* 2015, **112**, 8205-8210.