Supplementary Information

Large reduction of thermal conductivity leading to enhanced thermoelectric performance in p-type Mg_3Bi_2-$YbMg_2Bi_2$ solid solutions

Ting Zhou,[ab] Jun Mao,[b] Jing Jiang,[a] Shaowei Song,[b] Hangtian Zhu,[b] Qing Zhu,[b] Qinyong Zhang,[c] Wuyang Ren,[bd] Zhiming Wang,[d] Chao Wang,*[a] Zhifeng Ren*[b]

[a] State Key Laboratory of Electronic Thin Films and Integrated Devices, School of Electronic Science and Engineering, University of Electronic Science and Technology of China, Chengdu 611731, China. *E-mail: cwang@uestc.edu.cn

[b] Department of Physics and TcSUH, University of Houston, Houston, Texas 77204, United States. *E-mail: zren@uh.edu

[c] Key Laboratory of Fluid and Power Machinery of Ministry of Education, Center for Advanced Materials and Energy, Xihua University, Chengdu 610039, China.

[d] Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 610054, China.

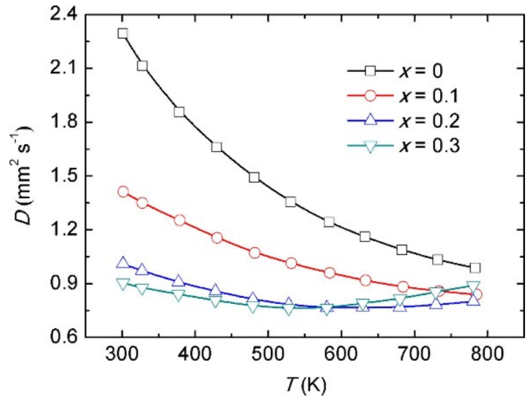

Fig. S1. Temperature-dependent diffusivity of $Yb_{1-x}Mg_xMg_2Bi_{1.96}$ (x = 0, 0.1, 0.2, and 0.3).

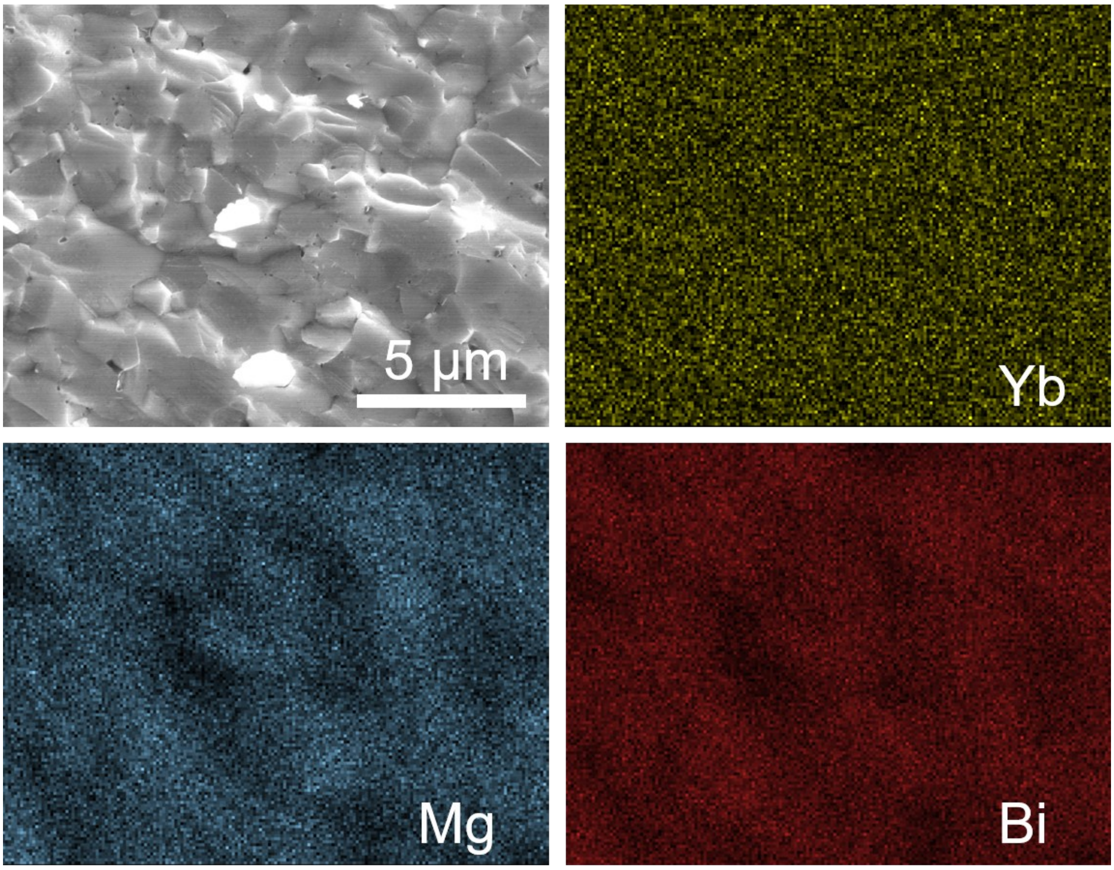

Fig. S2. Typical scanning electron microscopy image of the fractured surface morphology and the corresponding energy-dispersive X-ray spectroscopy mapping for the $Yb_{0.8}Mg_{0.2}Mg_2Bi_2$ sample.

Table S1. Theoretical density, experimental density, and relative density of $Yb_{1-x}Mg_xMg_2Bi_{1.96}$ (x = 0, 0.1, 0.2, and 0.3).

Composition	Theoretical density ($g\ cm^{-3}$)	Experimental density ($g\ cm^{-3}$)	Relative density
$YbMg_2Bi_{1.96}$	7.10	7.06	99.44%
$Yb_{0.9}Mg_{0.1}Mg_2Bi_{1.96}$	6.97	6.94	99.57%
$Yb_{0.8}Mg_{0.2}Mg_2Bi_{1.96}$	6.83	6.82	99.85%
$Yb_{0.7}Mg_{0.3}Mg_2Bi_{1.96}$	6.69	6.68	99.85%

Calculation of the Pisarenko plot:

The relationship between the Seebeck coefficient and the Hall carrier concentration (Pisarenko plot) is calculated by using the single parabolic band model with the assumption of an acoustic phonon scattering mechanism,[1, 2] based on eqns. (1)–(4):

$$S = \pm \frac{k_B}{e}\left(\frac{2F_1(\eta)}{F_0(\eta)} - \eta\right) \tag{1}$$

$$r_H = \frac{3}{2}\frac{F_{1/2}(\eta)F_{-1/2}(\eta)}{2F_0^2(\eta)} \tag{2}$$

$$F_n(\eta) = \int_0^\infty \frac{\chi^n}{1+e^{\chi-\eta}}d\chi \tag{3}$$

$$m^* = \frac{h^2}{2k_BT}\left[\frac{nr_H}{4\pi F_{1/2}(\eta)}\right]^{2/3}, \tag{4}$$

where $F_n(\eta)$ is the nth order Fermi integral, η is the reduced Fermi energy, r_H is the Hall factor, h is the Planck constant, k_B is the Bolzmann constant, e is the electron charge, and m^* is the total density of states effective mass.

References

1. S. Airapetyants, M. Vinogradova, I. Dubrovskaya, N. Kolomoets and I. Rudnik, *SOVIET PHYS SOLID STATE*, 1966, **8**, 1069-1072.
2. Z. Liu, H. Geng, J. Mao, J. Shuai, R. He, C. Wang, W. Cai, J. Sui and Z. Ren, *Journal of Materials Chemistry A*, 2016, **4**, 16834-16840.