Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supplementary Information

FeVSb-based amorphous films with ultra-low thermal conductivity and high *ZT*: a potential material for thermoelectric generators

Chenjin Liu[1], Yucheng Xiong[2], Yajie Huang[1], Xing Tan[1], Liangliang Li[1, 3]*, Dongyan Xu[2]*, Yuan-Hua Lin[1], Ce-Wen Nan[1]

[1]State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

[2]Department of Mechanical and Automation Engineering, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong Special Administrative Region, China

[3]Key Laboratory of Advanced Materials (MOE), School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Corresponding author e-mail: liliangliang@mail.tsinghua.edu.cn

Phone: +86-10-62797162

Fax: +86-10-62771160

Postal address: State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Corresponding author e-mail: dyxu@mae.cuhk.edu.hk

Phone: +852-39438045

Fax: +852-26036002

Postal address: Department of Mechanical and Automation Engineering, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong Special Administrative Region, China

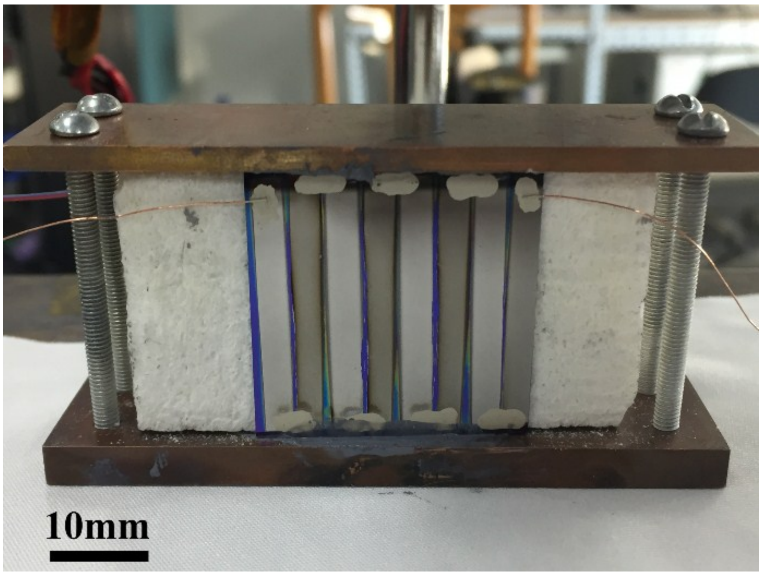

Figure S1. Photograph of the planar TEG placed between two Cu plates.

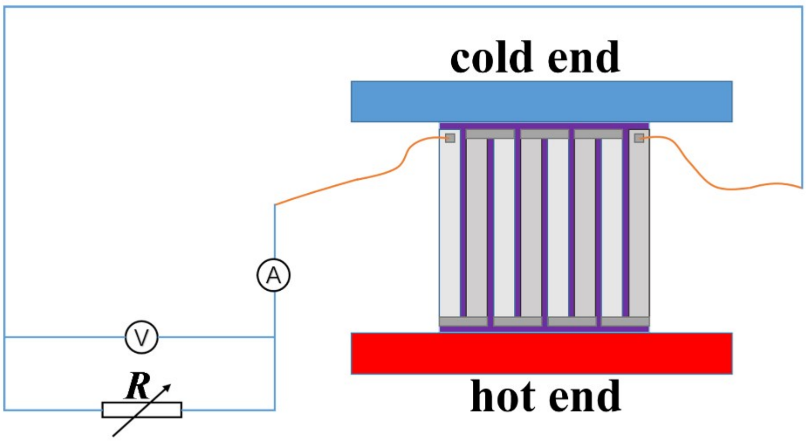

Figure S2. Circuit diagram to measure the TEG performance.

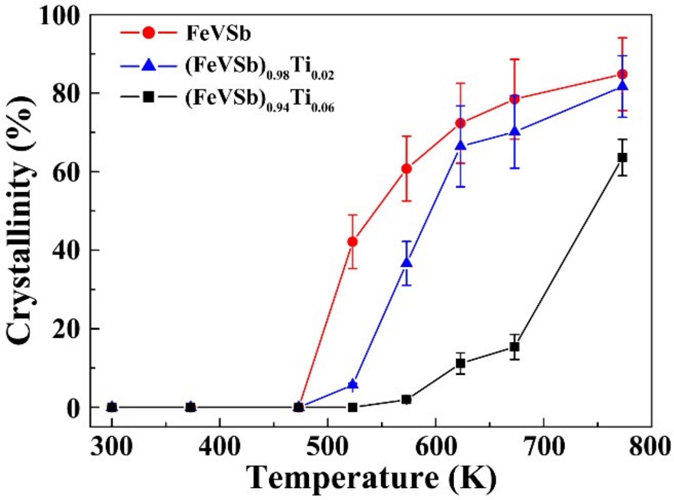

Figure S3. Crystallinity of FeVSb, $(FeVSb)_{0.98}Ti_{0.02}$, and $(FeVSb)_{0.94}Ti_{0.06}$ samples based on the in situ high temperature XRD data with the peak fitting method.

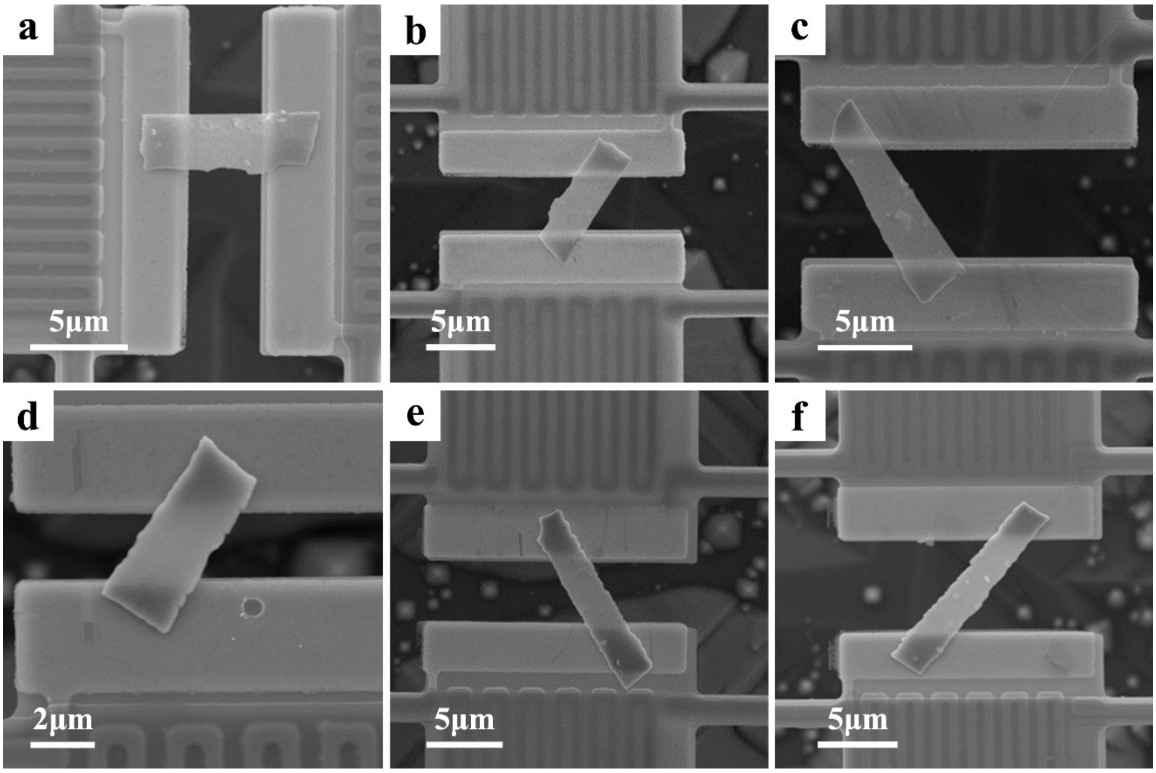

Figure S4. SEM images of the FeVSb (a–c) and $(FeVSb)_{0.94}Ti_{0.06}$ (d–f) samples with different suspended lengths L_s placed onto the microdevices, which are used to measure the thermal conductivity by the suspended thermal bridge method. (a) L_s=4.10 μm. (b) L_s=4.94 μm. (c) L_s=7.59 μm. (d) L_s=2.58 μm. (e) L_s=5.06 μm. (f) L_s=8.56 μm.

Uncertainty Analysis of Thermal Conductivity Measurement

Thermal conductivity is extracted from the measurements on the same sample with three different suspended lengths. For a uniform sample, the measured R_{tot} can be written as:

$$R_{tot} = R_c + R_{s/L} \times L_s, \quad (1)$$

where R_c is the contact thermal resistance between the sample and two membranes, $R_{s/L}$ is the thermal resistance per unit length, and L_s is the suspended length. R_c can be assumed as a constant in different measurements when the sample is fully thermalized with membranes at two ends according to the fin heat transfer model.[1] The insets of Figures 9a and 9b show that there is a good linear relationship between the R_{tot} and L_s for both samples, which in return verifies the assumption that the R_c is a constant in different measurements. The slope of the linear lines in the insets of Figures 9a and 9b stands for the $R_{s/L}$, thus the thermal conductivity κ is determined by

$$\kappa = 1/(w \cdot t \cdot R_{s/L}), \quad (2)$$

where w and t are the width and thickness of the sample, respectively.

The relative uncertainty in the extracted thermal conductivity can be calculated by

$$\frac{\delta\kappa}{\kappa} = \sqrt{\left(\frac{\delta R_{s/L}}{R_{s/L}}\right)^2 + \left(\frac{\delta w}{w}\right)^2 + \left(\frac{\delta t}{t}\right)^2}, \quad (3)$$

where $\delta R_{s/L}$, δw, and δt are the uncertainties in the thermal resistance per unit length, width, and thickness, respectively. The width w is determined from the SEM images and its uncertainty δw is estimated as 5 nm. The thickness t is measured by AFM and its uncertainty δt is estimated as 5 nm.

From the measurements on the thermal resistances (R_{tot}) at three different suspended lengths (L_s), the $R_{s/L}$ is determined by the least squares fitting,

$$R_{s/L} = \frac{n\sum_{i=1}^{n} L_{s,i} R_{tot,i} - \sum_{i=1}^{n} L_{s,i} \sum_{i=1}^{n} R_{tot,i}}{n\sum_{i=1}^{n} L_{s,i}^{2} - \left(\sum_{i=1}^{n} L_{s,i}\right)^{2}} \quad , \qquad (4)$$

where n is 3 in our measurements. Then, the uncertainty in $R_{s/L}$ is estimated by the following expression:[2]

$$\delta R_{s/L} = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial R_{s/L}}{\partial R_{tot,i}}\right)^{2} \delta R_{tot,i}^{2} + \sum_{i=1}^{n} \left(\frac{\partial R_{s/L}}{\partial L_{s,i}}\right)^{2} \delta L_{s,i}^{2}} \quad , \qquad (5)$$

where $\delta R_{tot,i}$ and $\delta L_{s,i}$ are the uncertainties in the measured thermal resistances and the suspended lengths, respectively. The relative uncertainty in the measured thermal resistance ($\delta R_{tot,i}/R_{tot,i}$) is evaluated using the Monte Carlo method and is less than 5% for the measured samples. The suspended length L_s is measured from the SEM images, and the error $\delta L_{s,i}$ is estimated to be 10 nm.

With the uncertainty data listed above, the uncertainty in the thermal conductivity $\delta\kappa$ can be calculated with Eq. (3). For example, the $\delta\kappa$ is 0.209 and 0.094 $Wm^{-1}K^{-1}$ for the FeVSb and $(FeVSb)_{0.94}Ti_{0.06}$ films at 300 K, respectively.

References:

1. C. H. Yu, S. Saha, J. H. Zhou, L. Shi, A. M. Cassell, B. A. Cruden, Q. Ngo and J. Li, *Journal of Heat Transfer-Transactions of the Asme*, 2006, **128**, 234-239.
2. H. W. Coleman and W. G. Steele, *Experimentation, Validation, and Uncertainty Analysis for Engineers, Third Edition*, 2009.