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

Supporting Information

New Insights into the Role of Dislocation Engineering in N-type Filled Skutterudite $CoSb_3$

Zihang Liu[1⊥], Xianfu Meng[1,2⊥], Dandan Qin[1], Bo Cui[1], Haijun Wu[3], Yang Zhang[3], Stephen J. Pennycook[3], Wei Cai[1] and Jiehe Sui[1*]

[1] State Key Laboratory of Advanced Welding and Joining, Harbin Institute of Technology, Harbin 150001, China

[2] Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621900, China

[3] Department of Materials Science and Engineering, National University of Singapore 117575, Singapore

* To whom correspondence should be addressed. E-mail: suijiehe@hit.edu.cn

⊥ Equal contributors

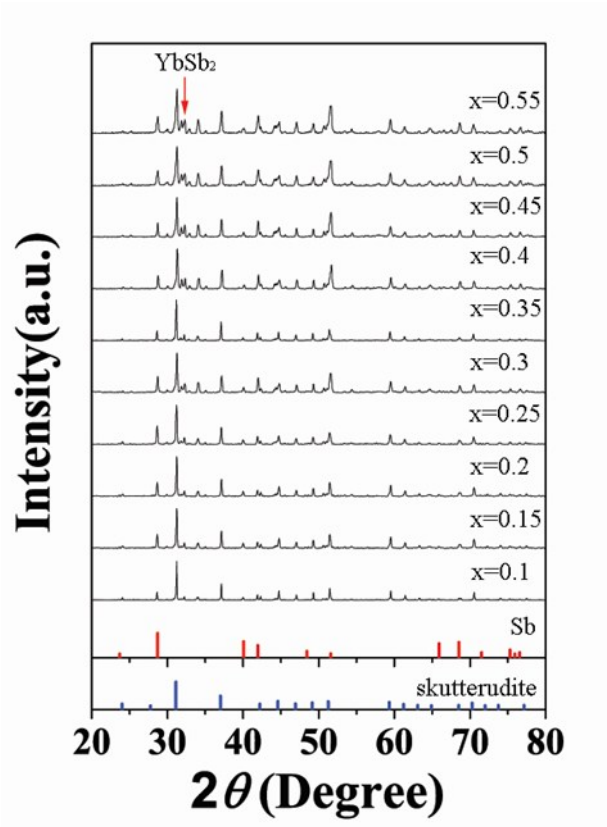

Figure S1 XRD patterns of $Yb_xCo_4Sb_{14.4}$ ribbons (x = 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5, and 0.55)

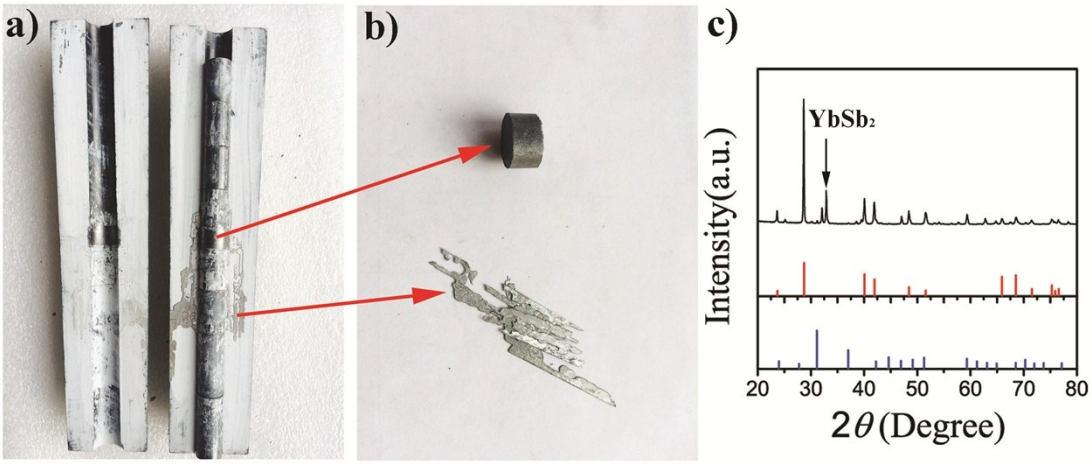

Figure S2 Images of compacted sample and expelled substance and XRD patterns of expelled substance. a) and b) Images of compacted sample and expelled substance, respectively. c) XRD patterns

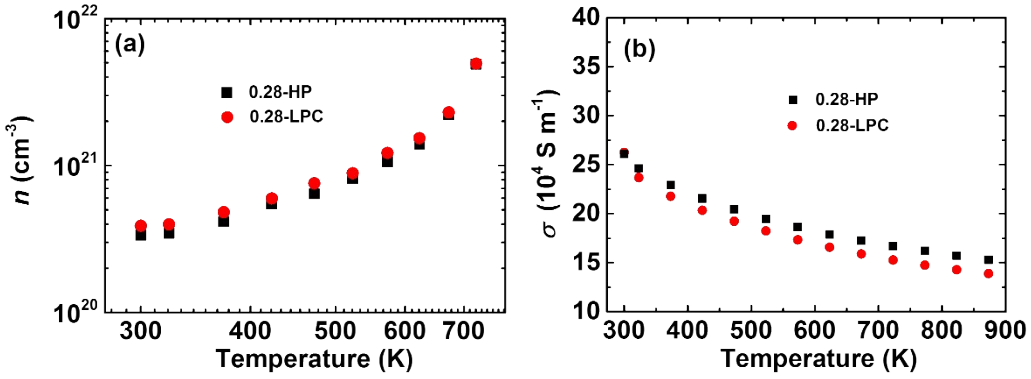

Figure S3 Temperature dependent (a) carrier concentration and (b) electrical conductivity for 0.28-HP and 0.28-LPC samples

Calculation of Debye temperature and Grüneisen parameter*:*

Both Debye temperature Θ_D and Grüneisen parameter γ can be calculated by the following equations based on the measured the longitudinal (v_l) and transverse (v_s) sound speed [1]:

$$v_a = \left(\frac{1}{3} \left[\frac{1}{v_l^3} + \frac{2}{v_s^3} \right] \right)^{-1/3} \tag{11}$$

$$\theta_D = \frac{h}{k_B} \left[\frac{3N}{4\pi V} \right]^{1/3} v_a \tag{12}$$

$$\varepsilon = \frac{2}{9} \left(\frac{6.4 \times \gamma (1 + \upsilon_p)}{(1 - \upsilon_p)} \right)^2 \tag{13}$$

$$\upsilon_p = \frac{1 - 2(v_s / v_l)^2}{2 - 2(v_s / v_l)^2} \tag{14}$$

$$\gamma = \frac{3}{2} \left(\frac{1 + \upsilon_p}{2 - 3\upsilon_p} \right) \tag{15}$$

where v_a is the average sound velocity, V the unit−cell volume, N the number of atoms in a unit cell, k_B the Boltzmann parameter, h the Planck constant, ε phenomenological adjustable parameter and υ_p the Poisson ratio.

[1] Y.-L. Pei, J. Q. He, J.-F. Li, F. Li, Q. J. Liu, W. Pan, C. Barreteau, D. Berardan, N. Dragoe, L.-D. Zhao, NPG Asia Mater. 2013, 5, e47.