Supporting Infomation

Enhanced Thermoelectric Properties in Pb-doped BiCuSeO Oxyselenides Prepared by Ultrafast Synthesis

Guang-Kun Ren,[a] *Jin-le Lan,*[b] *Sajid Butt,*[a,c] *Kyle J. Ventura,*[a] *Yuan-Hua Lin,*[a]* *Ce-Wen Nan*[a]

[a] State Key Laboratory of New Ceramics and Fine Processing, Tsinghua University, Beijing 100084, P. R. China

[b] College of Materials Science and Engineering, Beijing University of Chemical Technology, Beijing 100083, P. R. China

[c] Department of Materials Science and Engineering, Institute of Space Technology, Islamabad 44000, Pakistan

SHS process

The diameter of the cold-pressed pellet is 20mm, shown in Fig. S1. After SHS, the sample expanded and cracked (see inset graph in Fig. S1).

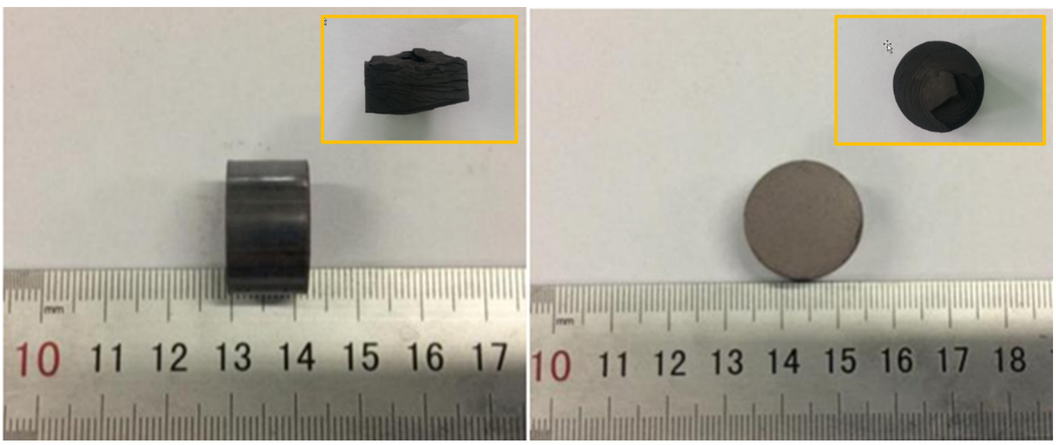

Fig. S1 The size of cold-pressed pellet before and after SHS

Thermal analysis

For the entire range of the DSC curve, we find there are no other peaks after 550K, which meant the composition reacted completely at the 75K min^{-1} heating rate. The curve is shown in Fig. S2. Cyclic thermal analysis suggests that the SHSed powder does not have any phase transition and its weight loss is within the system's error range (see graph Fig. S3), which indicates that the powder reacts completely from 323K to 973K.

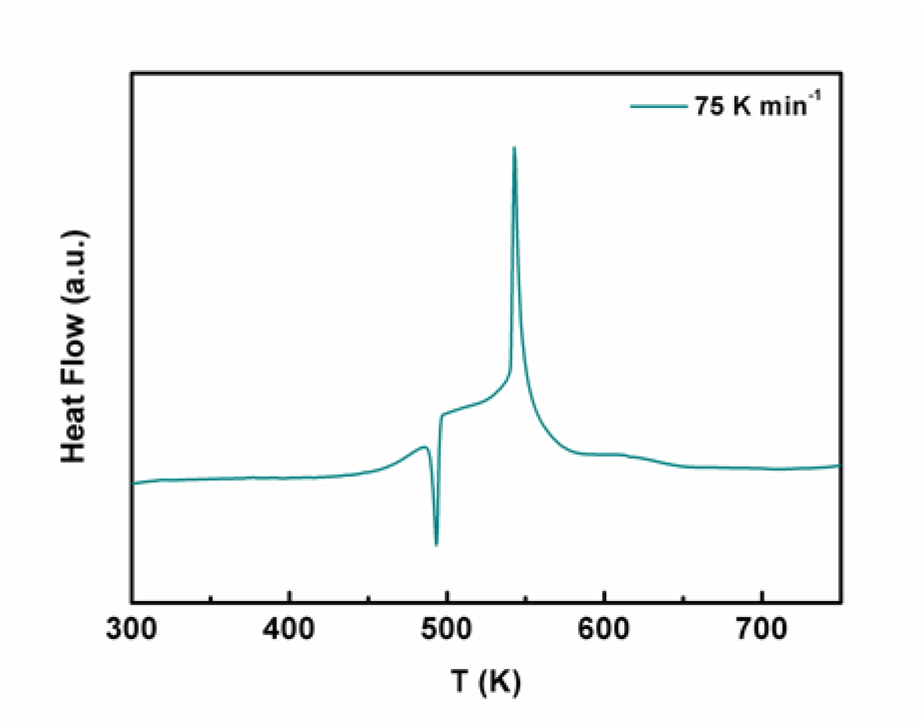

Fig. S2 DSC curve of the SHS process with 75K min^{-1}

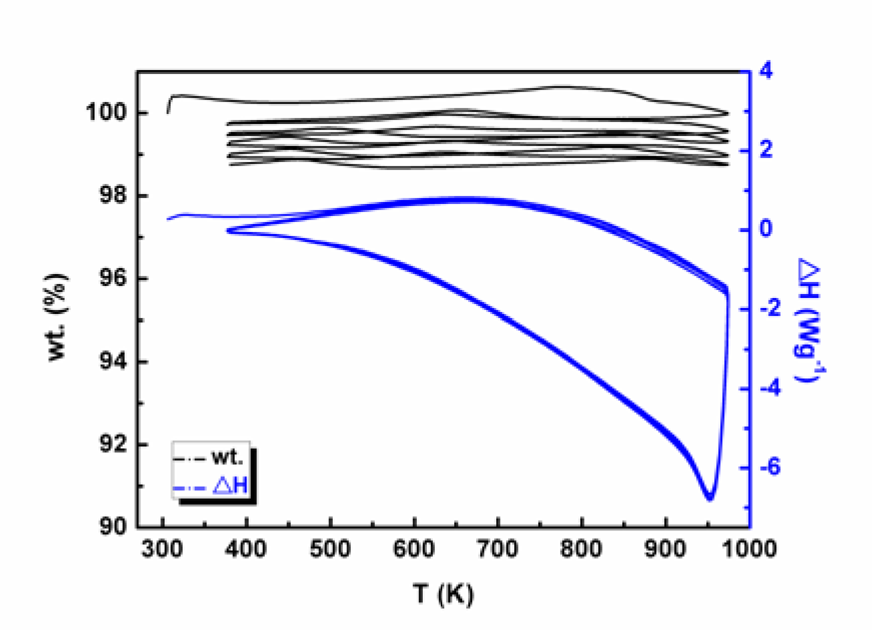

Fig. S3 Cyclic thermal analysis of powder synthesized by SHS.

Lorenz number and effective mass

In order to analyze the transport properties of samples, we measured their carrier concentration and mobility by Hall effect system, and based on single band model and electron-phonon interaction, the Lorenz number (see graph Fig. S4) and the effective mass can be expressed as follow (the effective mass depends on the reduced Fermi energy η decreases with increasing temperature):

$$S = \pm \frac{k_B}{e}\left(\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)} - \eta\right) \tag{1}$$

$$n = \frac{1}{2\pi^2}\left(\frac{2m^* k_B T}{\hbar^2}\right)^{3/2} F_{1/2}(\eta) \tag{2}$$

$$F_i(\xi) = \int_0^\infty \frac{x^i dx}{1+e^{x-\xi}} \tag{3}$$

$$L = \left(\frac{k_B}{e}\right)^2 \left(\frac{(r+7/2)F_{r+5/2}(\eta)}{(r+3/2)F_{r+3/2}(\eta)} - \left[\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)}\right]^2\right) \tag{4}$$

where e is the electronic charge, F_i is the Fermi integrals, and $\eta = E_F / k_B T$ is the reduce Fermi level, E_F is the electron Fermi level measured upward from the band edge. Meanwhile, acoustic phonon scattering ($r = -1/2$) has been assumed as the main carrier scattering mechanism. The effective mass is calculated by Equation (1-3). The Lorenz number can be obtained by applying the calculated reduced Fermi energy η and scattering parameter r into Equation (4).[1]

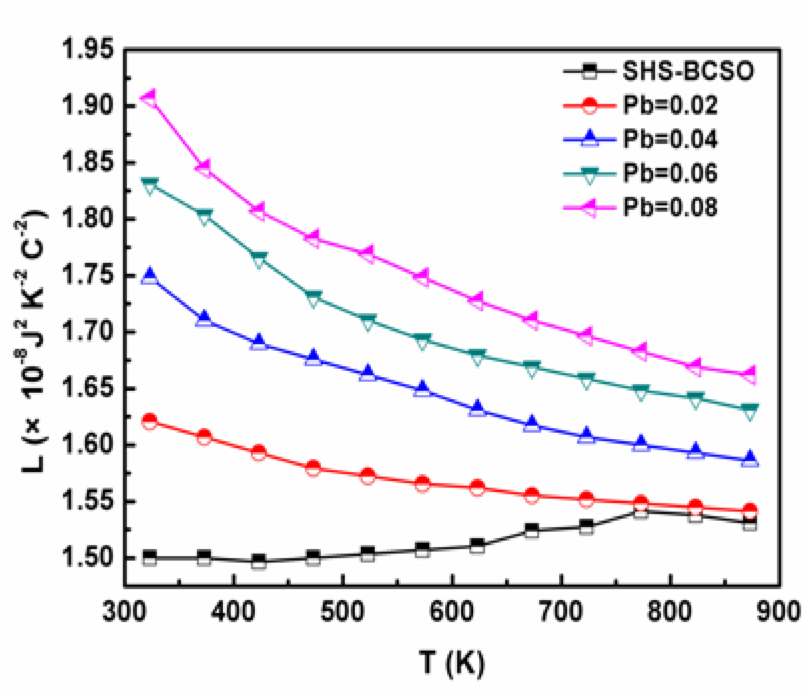

Fig. S4 The calculated Lorenz number based on single band model and electron-phonon interaction

Ref:

1. J. L. Lan, Y. C. Liu, B. Zhan, Y. H. Lin, B. Zhang, X. Yuan, W. Zhang, W. Xu and C. W. Nan, Adv. Mater., 2013, 25, 5086-5090.