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

Supporting Information

Cation disorder and thermoelectric properties in layered ternary compounds MBi_2Te_4 (M=Ge, Sn)

Hu Zhang[a,b], Lu Lu[c], Shaobo Mi[*a,b]

[a]*State Key Laboratory for Mechanical Behavior of Materials & School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China*

[b]*Ji Hua Laboratory, Foshan, 510006, Guangdong, China*

[c]*The Key Lab of Micro-nano Electronics and System Integration of Xi'an City &School of Microelectronics, Xi'an Jiaotong University, Xi'an 710049, China*

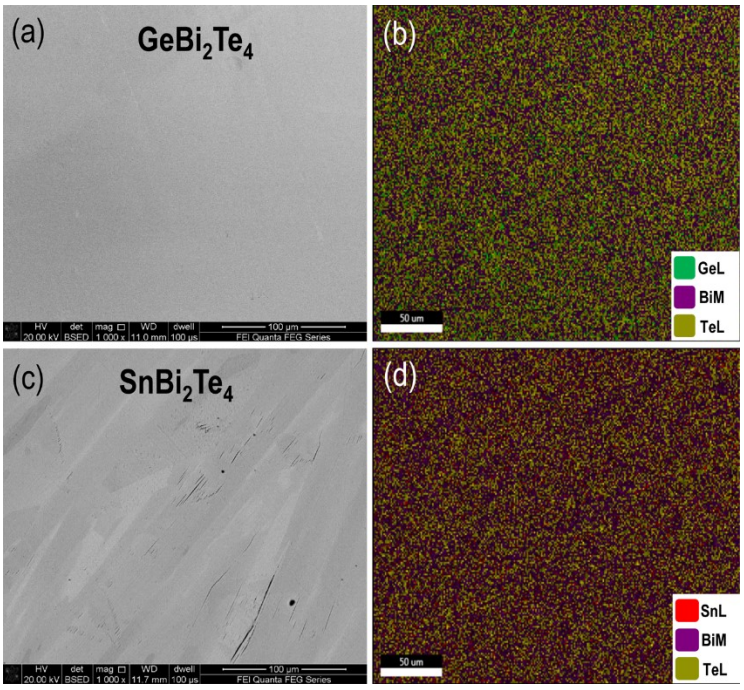

Fig. S1 Backscattered electron (BSE) images and elemental maps of $GeBi_2Te_4$ and $SnBi_2Te_4$ obtained in scanning electron microscope (SEM). The BSE-SEM images

* E-mail: shaobo.mi@xjtu.edu.cn
Fax: +86 (29) 83395679
Tel: +86 (29) 83395023

displayed in (a) and (c) show a morphology of $GeBi_2Te_4$ and $SnBi_2Te_4$ samples. The contrast appeared in (a) and (c) results from the grains of different orientations. The corresponding elemental maps of $GeBi_2Te_4$ and $SnBi_2Te_4$ samples presented in (b) and (d) indicate a homogeneous distribution of constituent elements (Ge, Sn, Bi, and Te) in the samples.

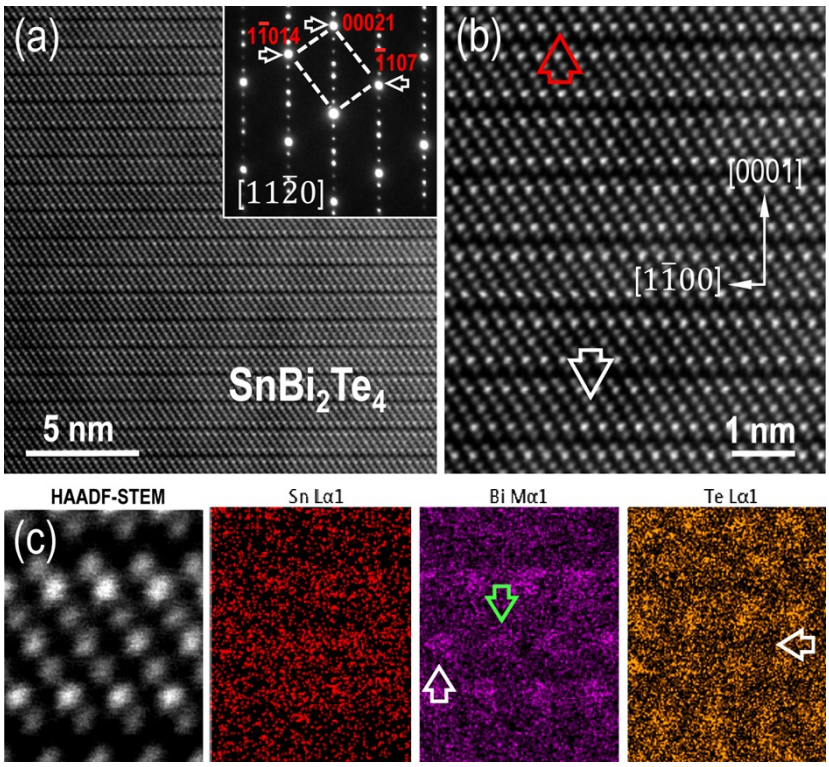

Fig. S2 The cation disorder in $SnBi_2Te_4$. (a, b) HAADF-STEM images of $SnBi_2Te_4$ viewed along the $[11\bar{2}0]$ zone axis. The insert in (a) is the corresponding SAED pattern. In (b), the intensity variation in the 3*a* site occupied by Sn, and the 6*c* site occupied by Bi is demonstrated by a vertical white arrow and a vertical red arrow, respectively. (c) HAADF-STEM image and the atomically resolved EDS maps of Sn-Lα1, Bi-Mα1, and Te-Lα1 of the $SnBi_2Te_4$ sample viewed along the $[11\bar{2}0]$ zone axis. The intensity fluctuation can be visible in the 3*a* site, as displayed by a vertical white arrow and a vertical green arrow, indicating the substitution of Sn cations by Bi cations in different ratios. The atomic plane of the 3*a* site is marked by a horizontal white arrow.