Electronic Supplementary Material (ESI)

Medium-temperature thermoelectric GeTe: vacancy suppression and band structure engineering leading to high performance

Jinfeng Dong[a], Fu-Hua Sun[a], Huaichao Tang[a], Jun Pei[b], Hua-Lu Zhuang[a], Hai-Hua Hu[a], Bo-Ping Zhang[b], Yu Pan[a,c], Jing-Feng Li[a]*

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

[b]The Beijing Municipal Key Laboratory of New Energy Materials and Technologies, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, 100083, China.

[c]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, Dresden 01187, Germany

* Corresponding authors. Emails: jingfeng@mail.tsinghua.edu.cn.

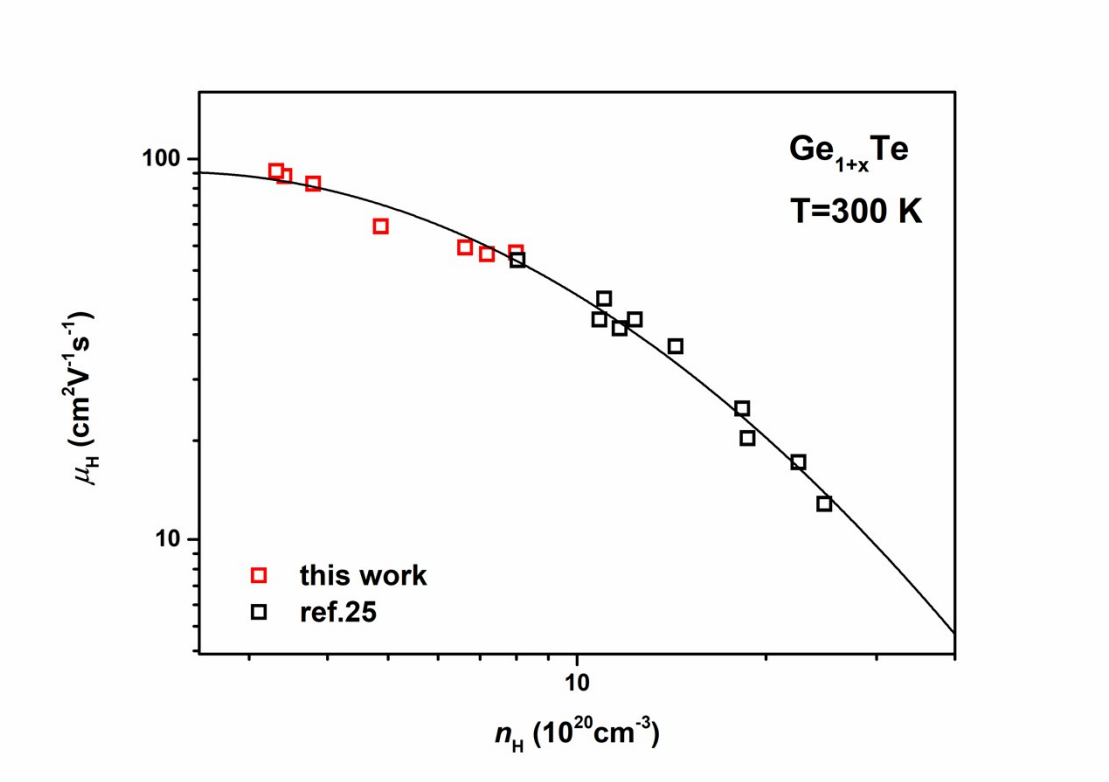

Fig.S1 Hole carrier concentration dependence of mobility at room temperature.

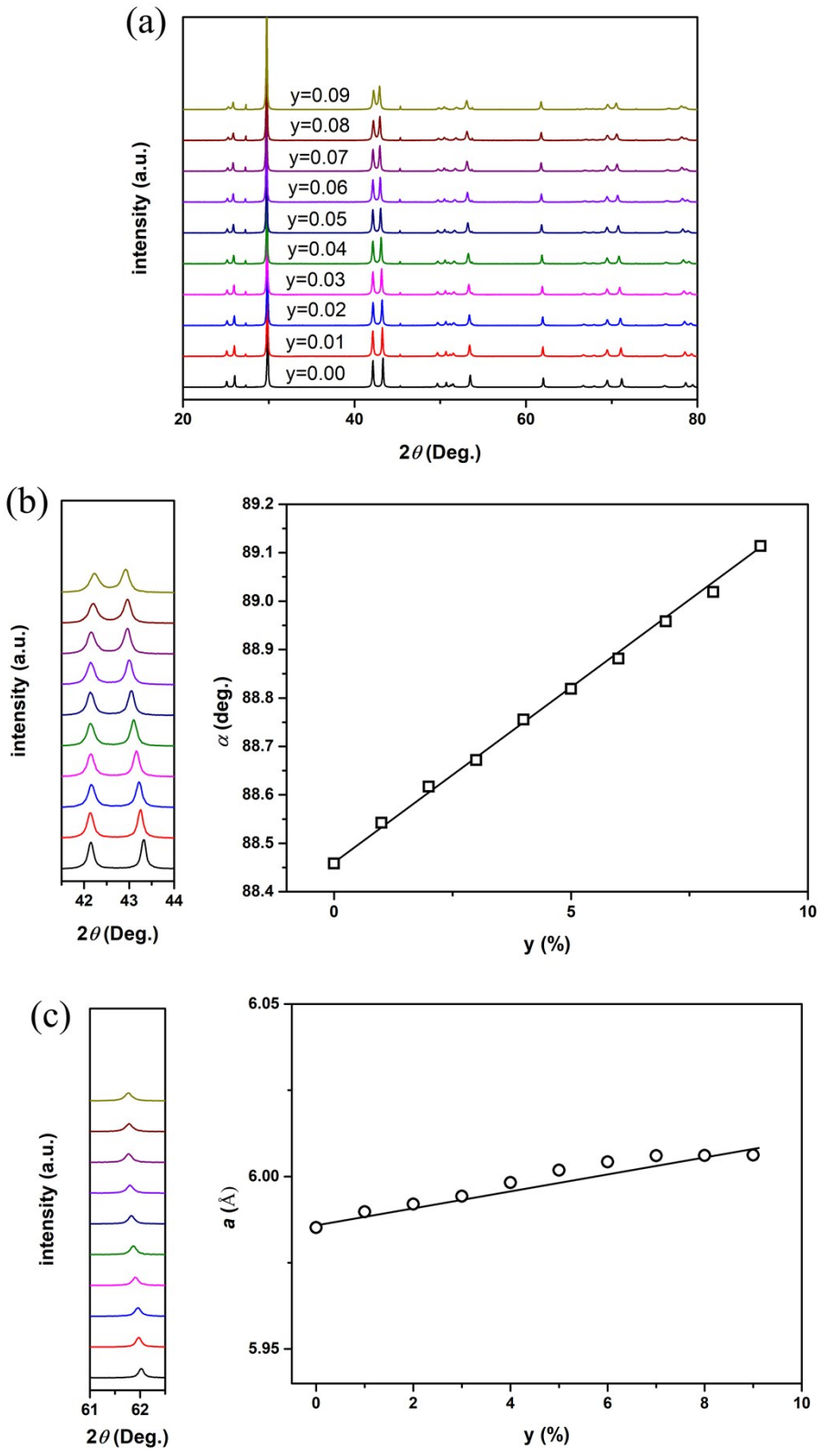

Fig.S2 (a) PXRD pattern of $Bi_yGe_{1.04-y}Te$. (b) enlarged XRD peaks between 42 – 44° and relationship between content of Bi and angle. (c) enlarged XRD peaks between 61 – 63° and the Bi content dependence of lattice parameter.

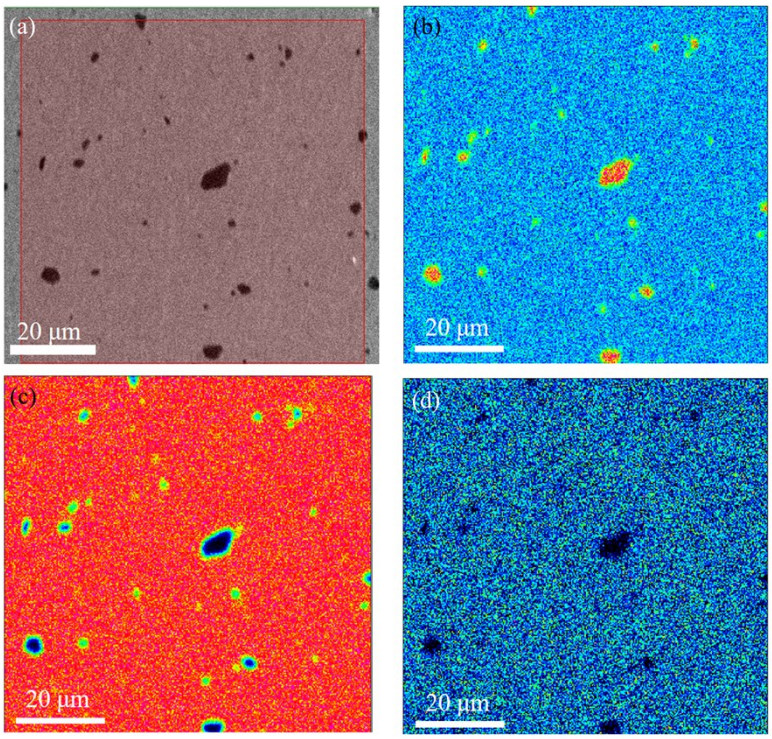

Fig.S3 (a) Polished surface morphologies of $Bi_{0.05}Ge_{0.99}Te$. (b) Ge (c) Te and (d) Bi mapping.

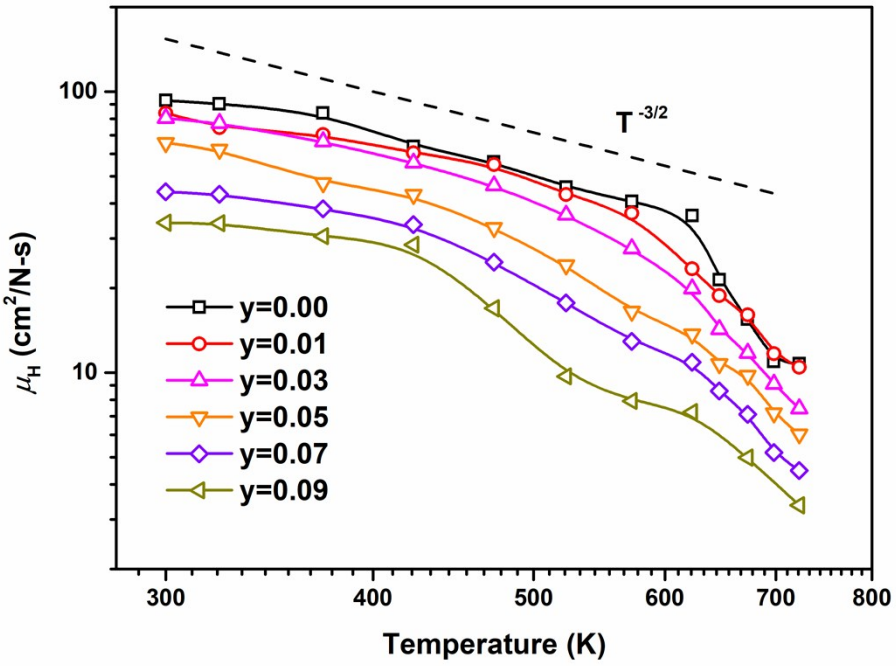

Fig.S4 Temperature dependent of Hall mobility for $Bi_yGe_{1.04-y}Te$.

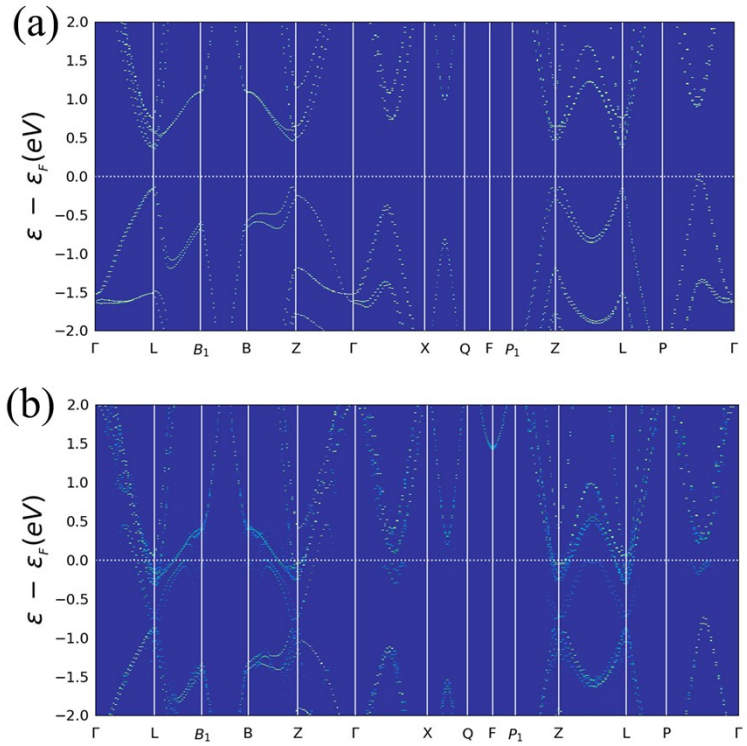

Fig.S5 Band structure of (a) pure rhombohedral GeTe (b) Bi doped rhombohedral GeTe (a 2x2x2 supercell was applied and one Ge atom was replaced by one Bi atom).

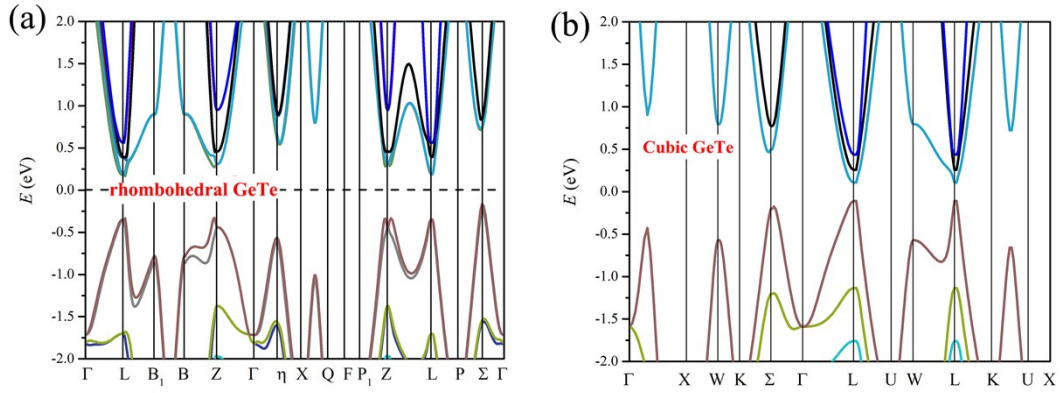

Fig.S6 Band structure of (a) rhombohedral GeTe (b) cubic GeTe.

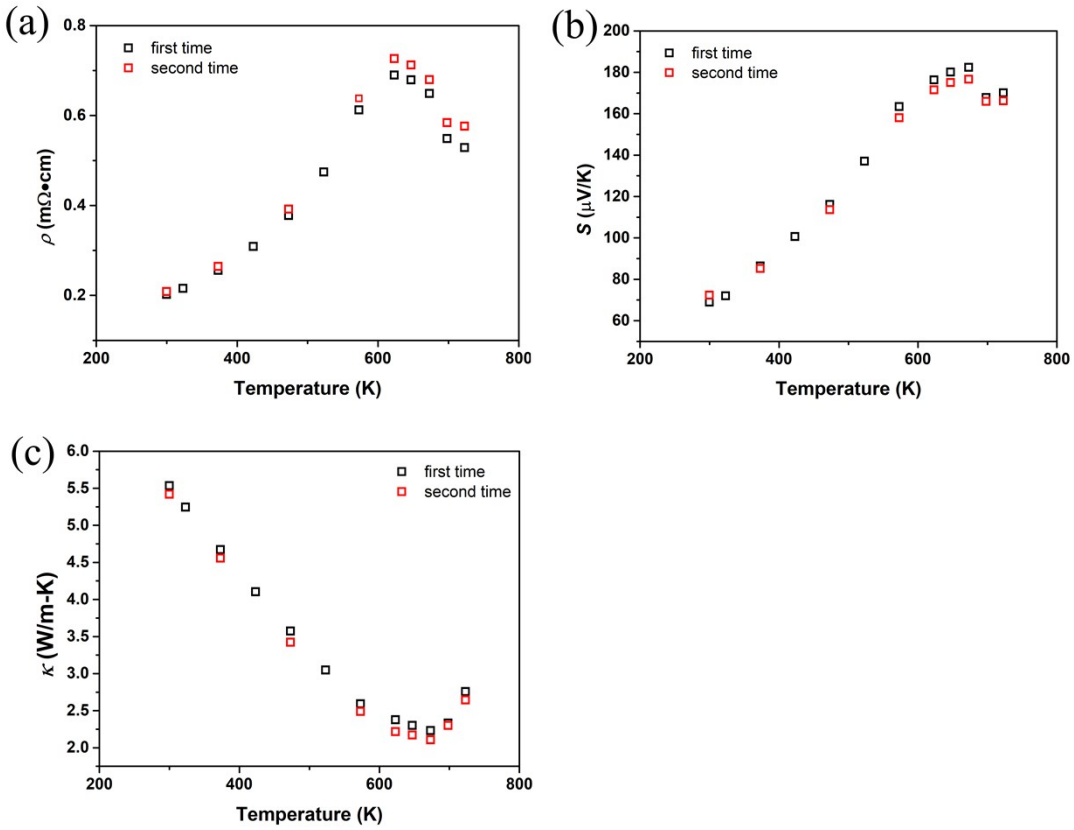

Fig.S7 Repeat measurement of (a) electrical resistivity, (b) Seebeck coefficient and (c) thermal conductivity of $Ge_{1.04}Te$.

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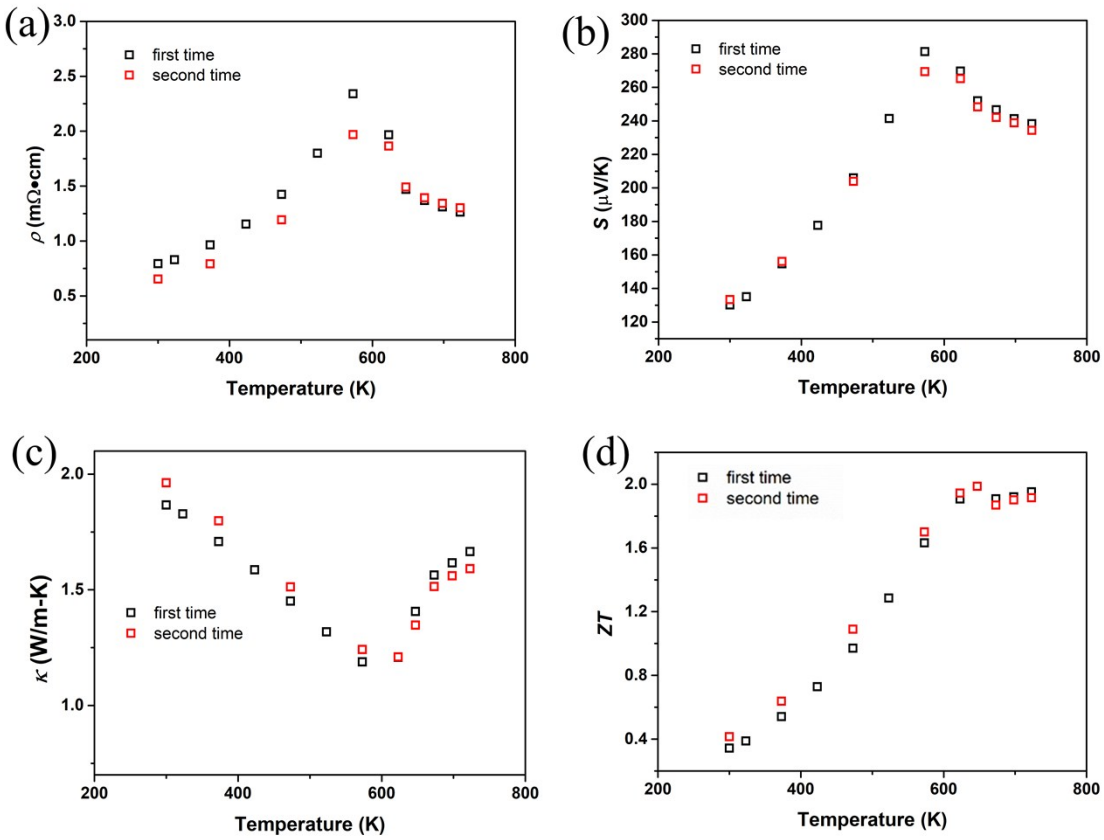

Fig.S8 Repeat measurement of (a) electrical resistivity, (b) Seebeck coefficient, (c) thermal conductivity and (d) calculated *ZT* value of $Bi_{0.05}Ge_{0.99}Te$.