Supplementary Information for

Anisotropic Thermoelectric Properties of GeTe Single Crystal

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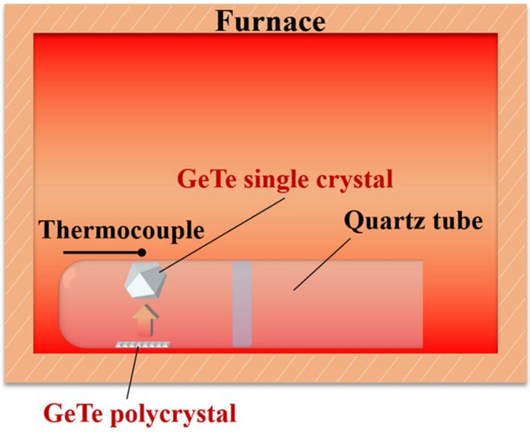

Fig. S1 Schematic of the growth of GeTe single crystal by heterogeneous chemical reaction.

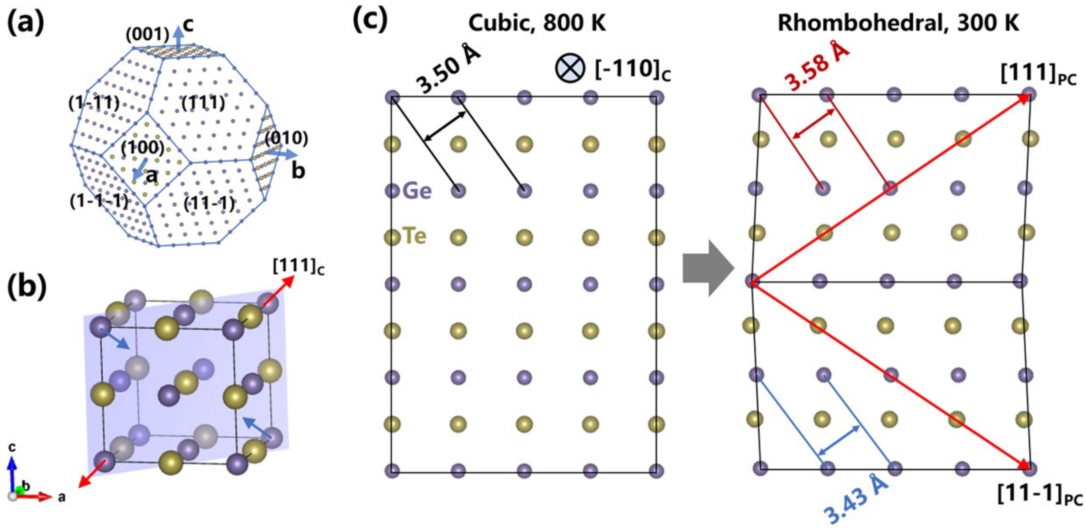

Fig. S2 Schematic of (a) the complete GeTe single crystal, (b) distortion of cubic cell along $[111]_{C}$ direction, (c) change of lattice spacings after lattice distortion along $[111]_{PC}$ and $[11\text{-}1]_{PC}$ directions.

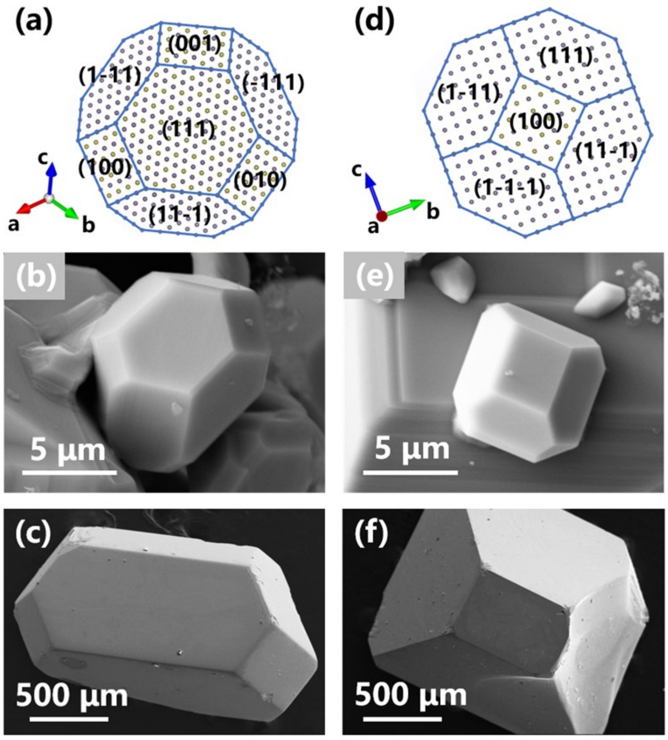

Fig. S3 Schematic and SEM images of GeTe single crystal with (a) (b) (c) hexagonal upper surface and (d) (e) (f) rectangular upper surface.

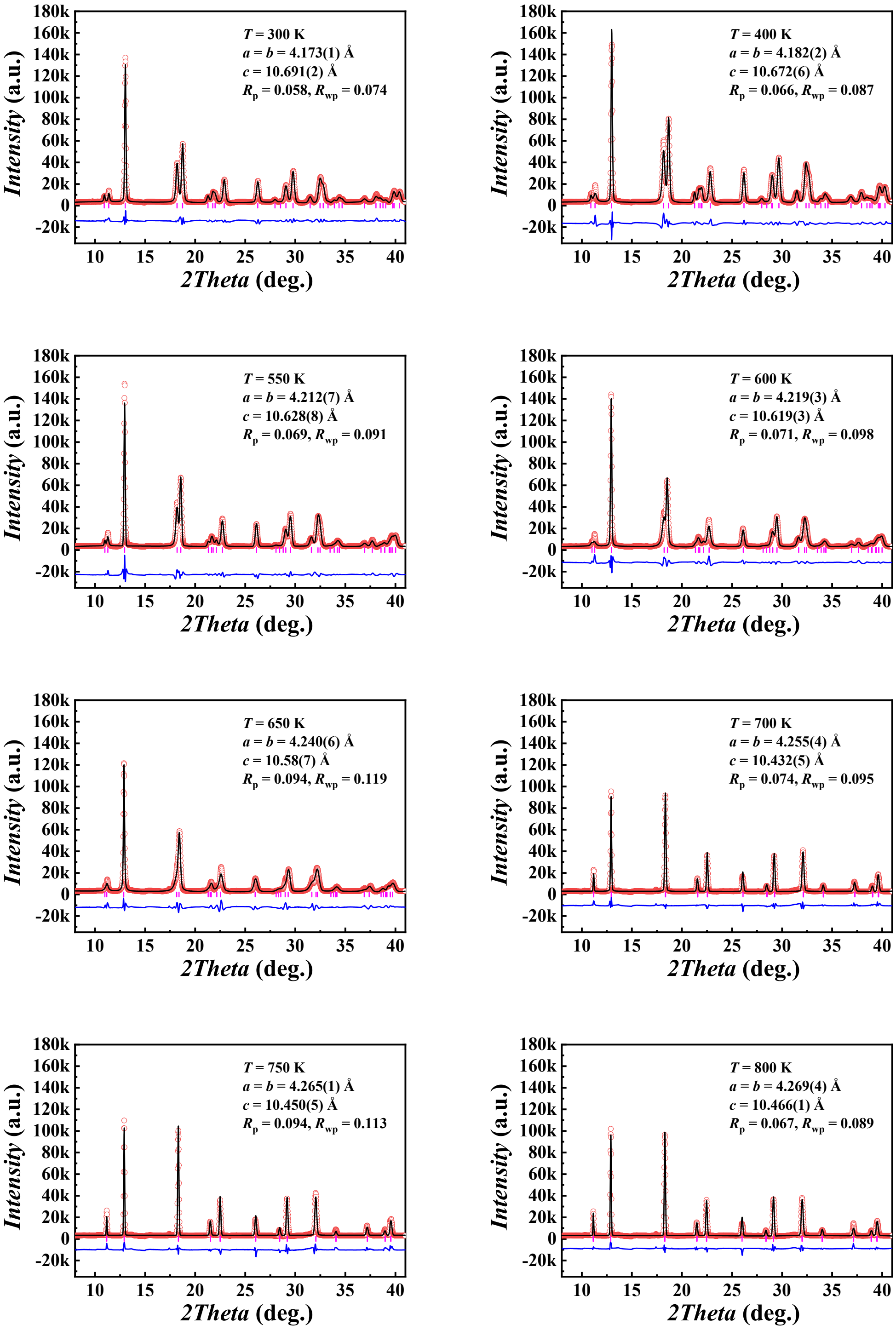

Fig. S4 Rietveld refinement for GeTe.

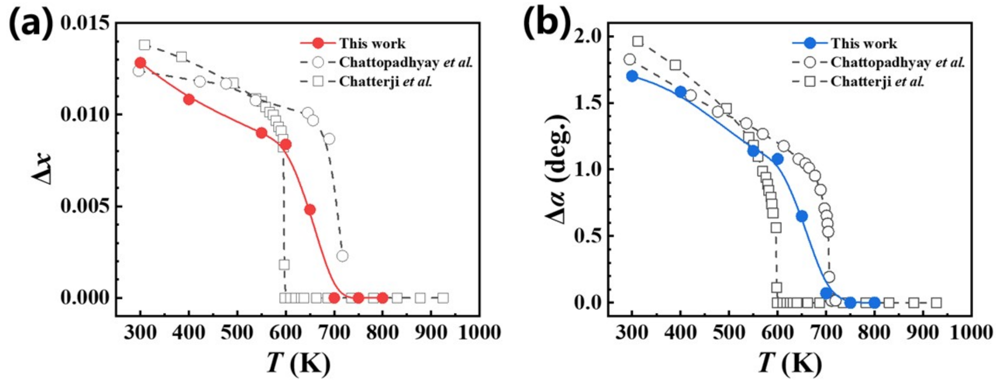

Fig. S5 Temperature variations of (a) distortion parameter Δx and (b) deviation $\Delta\alpha$ of the distortion angle from 90°. Comparisons with neutron diffraction experiments performed on GeTe single crystals by Chattopadhyay[2] and GeTe powder by Chatterji[3] are shown. All the continuous lines are just guides to the eye.

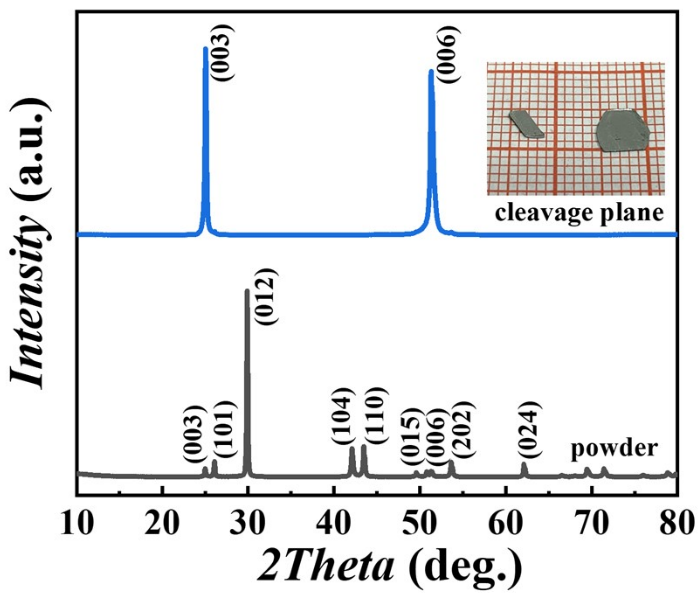

Fig. S6 XRD pattern of cleavage plane shows that the crystal orientation is $[001]_R$.

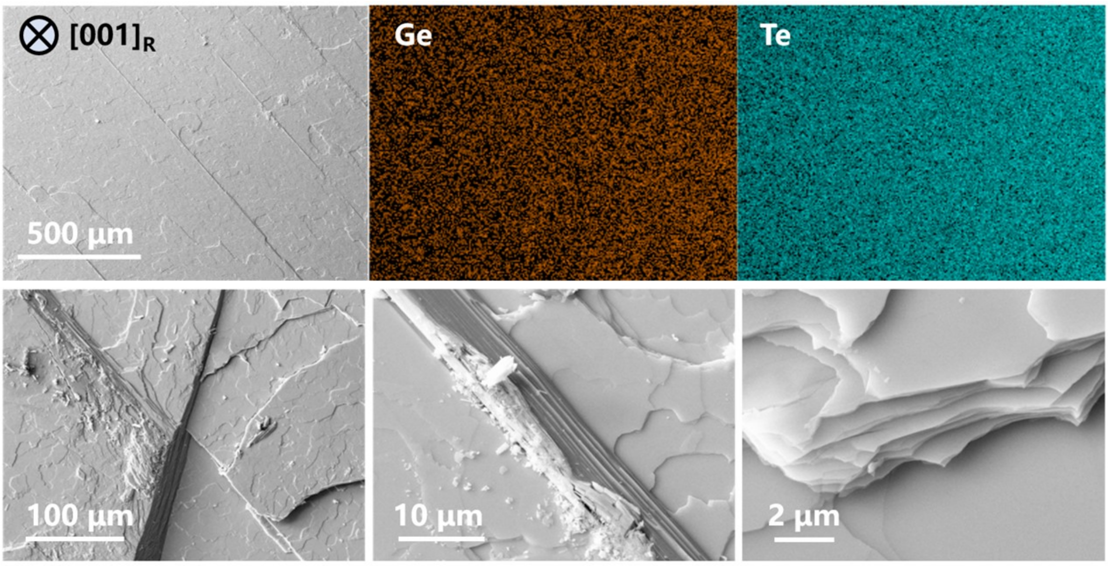

Fig. S7 SEM and EDS mapping images of cleavage plane show the lamellar morphology.

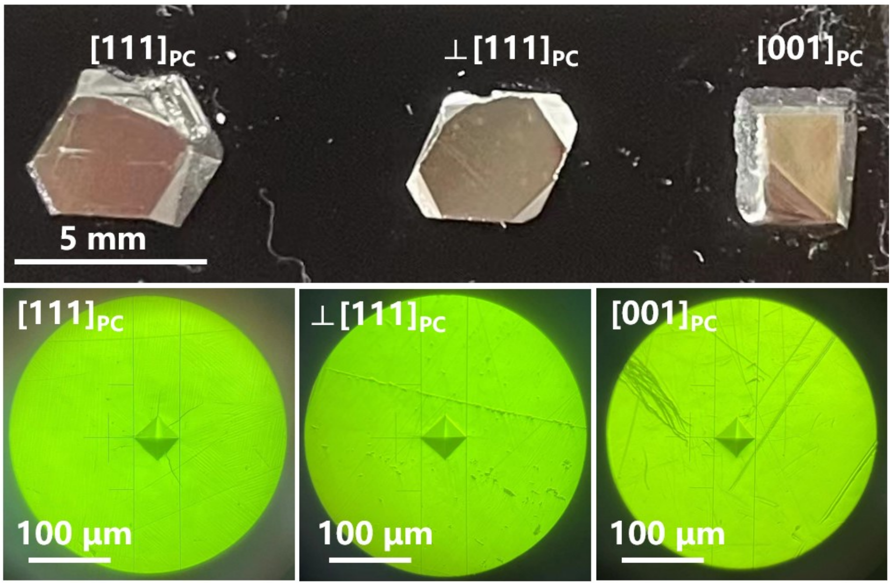

Fig. S8 Vickers microhardness measured on $[111]_{PC}$, $\perp[111]_{PC}$, and $[001]_{PC}$ planes, respectively.

Table S1 Vickers hardness on $[111]_{PC}$, $\perp[111]_{PC}$, $[001]_{PC}$ planes, and comparison with polycrystal.

Plane	$[111]_{PC}$	$\perp[111]_{PC}$	$[001]_{PC}$	polycrystal
Vickers hardness (HV)	122.2 ± 0.2	130.0 ± 1.7	140.1 ± 1.7	140.3 ± 1.6

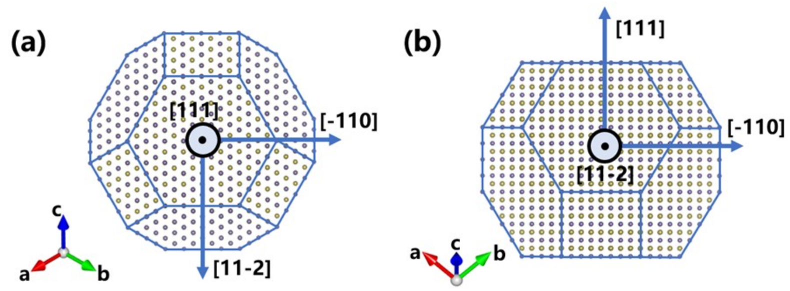

Fig. S9 Schematic of GeTe single crystals viewed in the [111] and [11-2] directions, respectively.

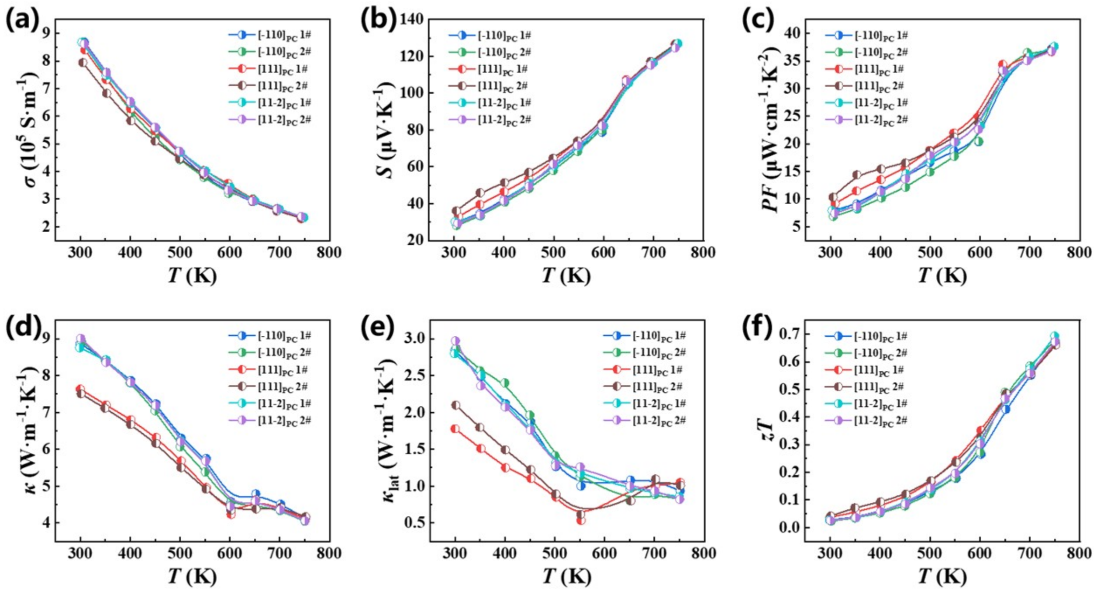

Fig. S10 Repeatability of thermoelectric properties. Temperature dependence of (a) electrical conductivity, (b) Seebeck coefficient, (c) power factor, (d) total thermal conductivity, (e) lattice thermal conductivity and (f) figure of merit zT of GeTe single crystal along the $[111]_{pc}$ and $\perp[111]_{pc}$ directions, where the $[-110]_{pc}$ and $[11\text{-}2]_{pc}$ are two orthogonal $\perp[111]_{pc}$ directions.

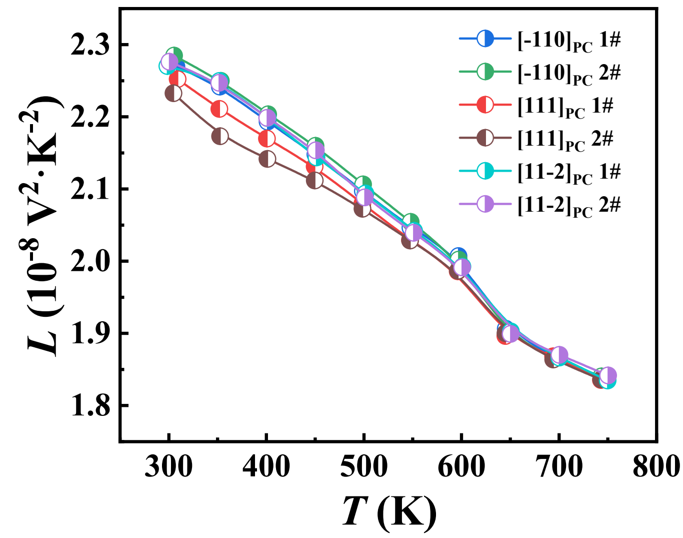

Fig. S11 Calculated Lorenz number of GeTe single crystal.

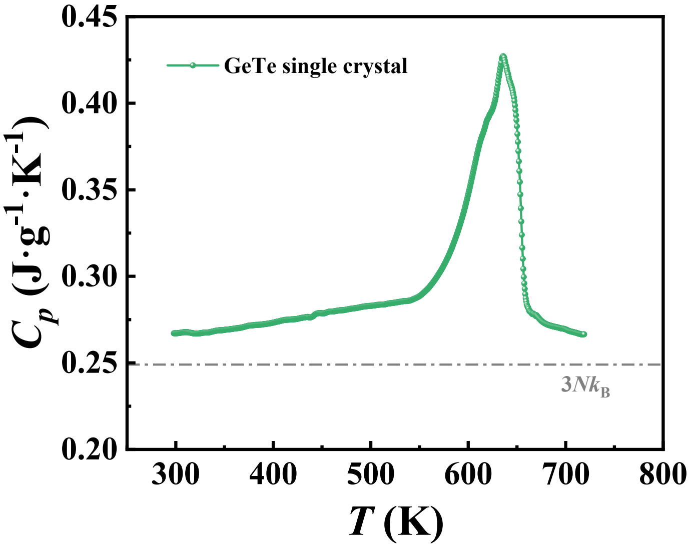

Fig. S12 Experimental heat capacity of GeTe single crystal.

References

1. G. Dhanaraj, K. Byrappa, V. Prasad and M. Dudley, *Springer Handbook of Crystal Growth*, Springer-Verlag Berlin Heidelberg, 2010.
2. T. Chattopadhyay, J. X. Boucherle and H. G. Vonschnering, *J. Phys. C Solid State*, 1987, **20**, 1431-1440.
3. T. Chatterji, C. M. N. Kumar and U. D. Wdowik, *Phys. Rev. B*, 2015, **91**, 054110.