

Supporting information

Impurity Band Engineering and Hierarchical Defect Scattering Enable High zT in Co-Doped AgSbTe_2

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1. Table S1 shows the elemental distribution of 3 regions in Figure 4e

Table S1 EDS Elemental Quantitative Analysis at region 1, 2, and 3 of $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ sample in Figure 4e.

| Region | Composition | Ag % | Sb % | Te % | Co % |
|--------|--|-------|-------|-------|-------|
| 1 | $\text{Co}_{2.60}\text{Sb}_2\text{Te}_{3.64}$ | 0 | 24.28 | 44.15 | 31.56 |
| 2 | $\text{Ag}_{4.71}\text{Sb}_{0.05}\text{Co}_{0.04}\text{Te}_3$ | 60.36 | 0.70 | 38.41 | 0.53 |
| 3 | $\text{Ag}_{1.04}\text{Sb}_{0.93}\text{Co}_{0.036}\text{Te}_2$ | 26.25 | 23.35 | 50.31 | 0.09 |

2. Figure S1 shows the TEM image and related EDS map of $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ sample, which confirms that cobalt was doped into the matrix and their Sb-rich and Ag-rich secondary phases.

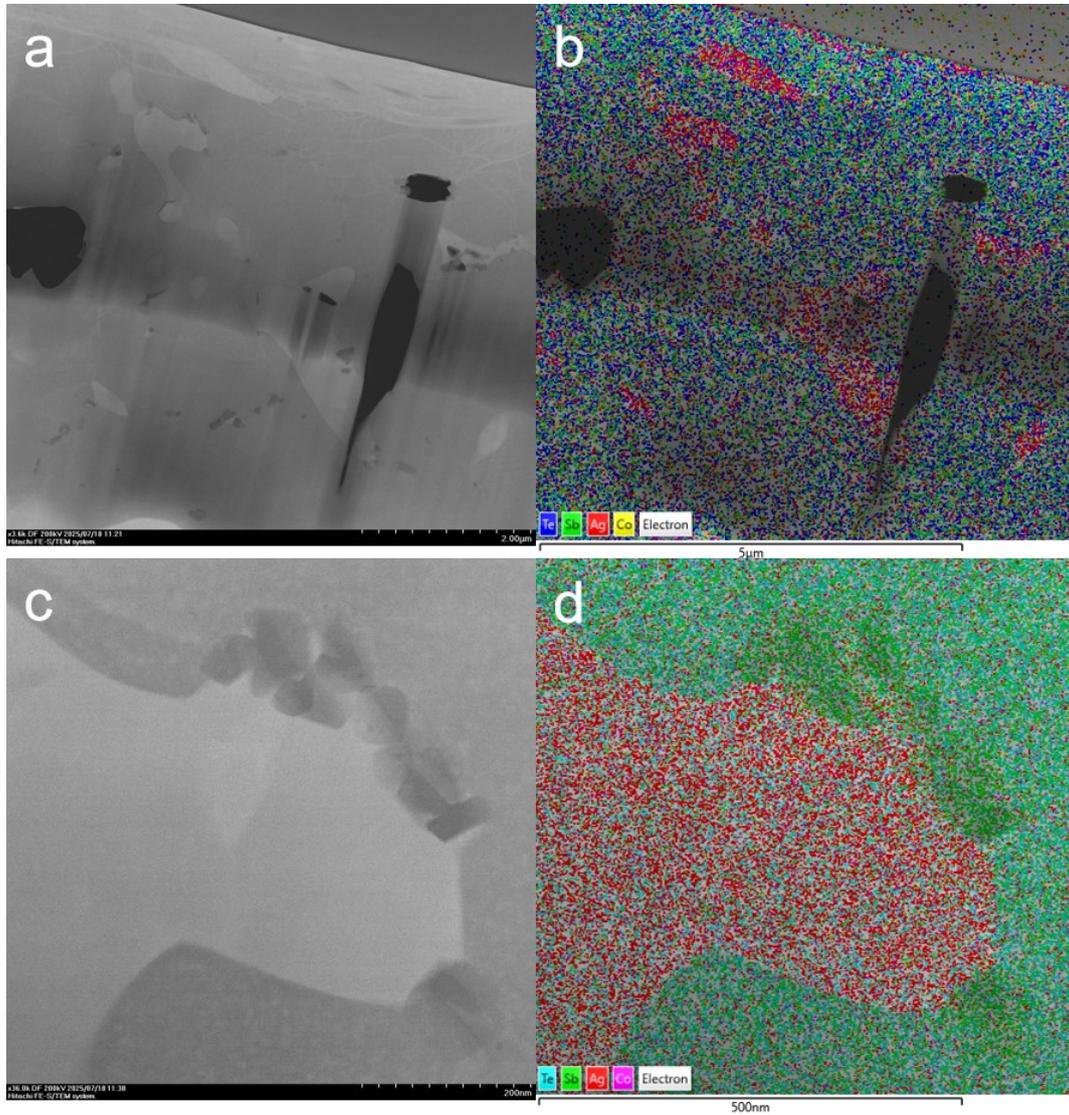


Figure S1 TEM images of $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ and their relative EDS maps.

3. Figure S2 shows the TEM images of defects in $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ sample.

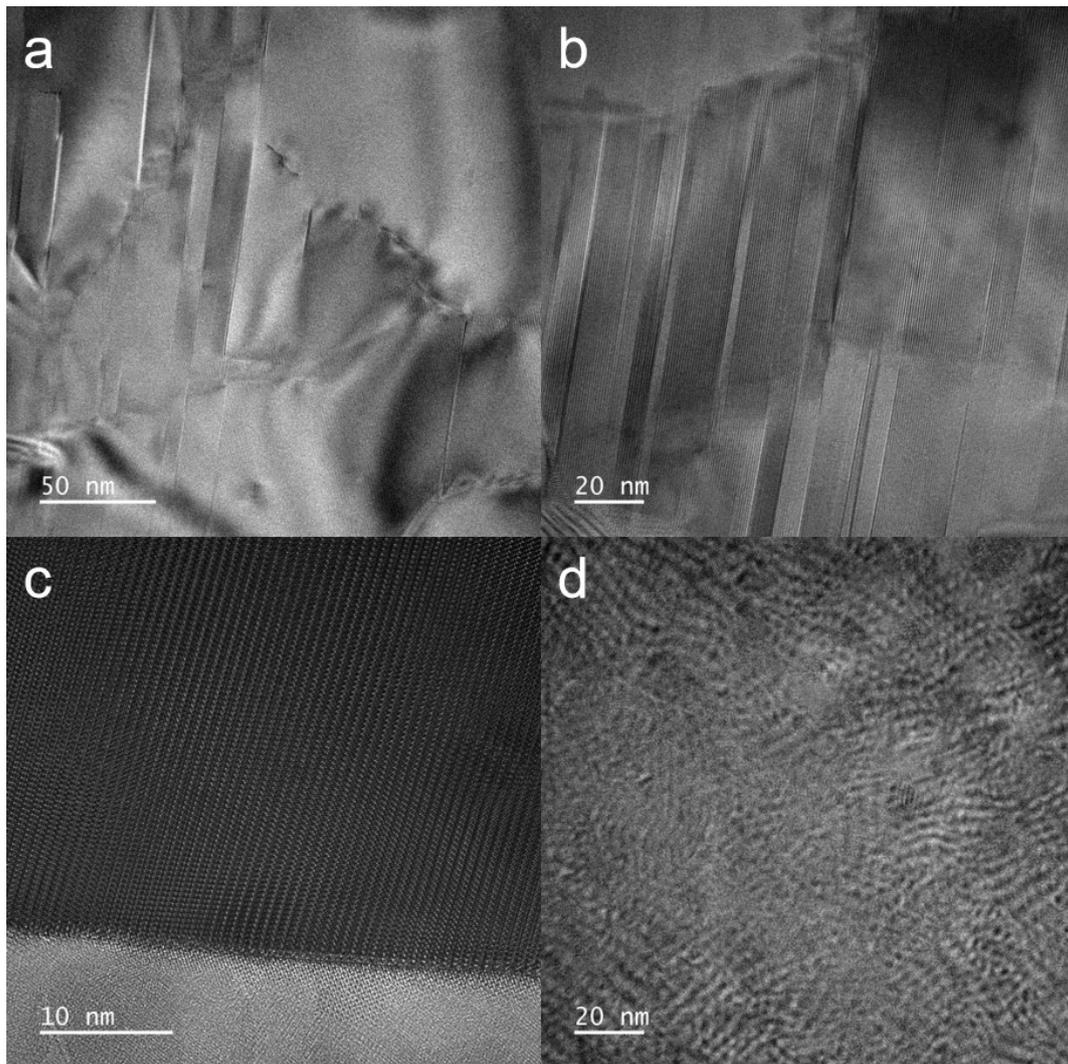


Figure S2 TEM images of defects in $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ sample.

4. Figure S3 shows the calculated weighted moility of $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ sample.

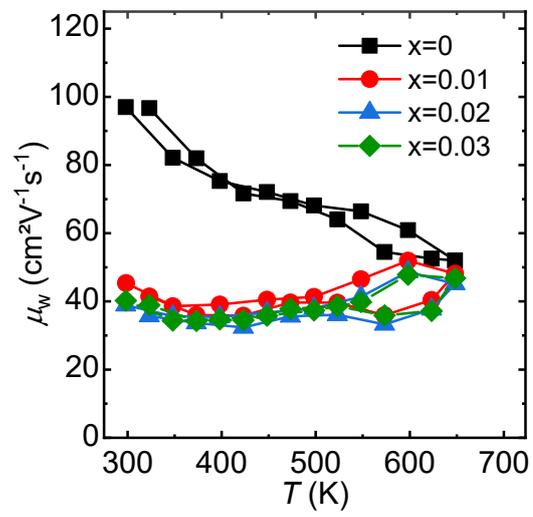


Figure S3 calculated weighted moility of $\text{AgSb}_{0.97}\text{Co}_{0.03}\text{Te}_2$ sample.

5. Figure S4 and Table S2 shows the Rietveld refinement of the XRD pattern of AgSbTe_2 with CoTe_2 (a) and $\text{CoSb}_{0.5}\text{Te}_{1.5}$ (b) secondary phase.

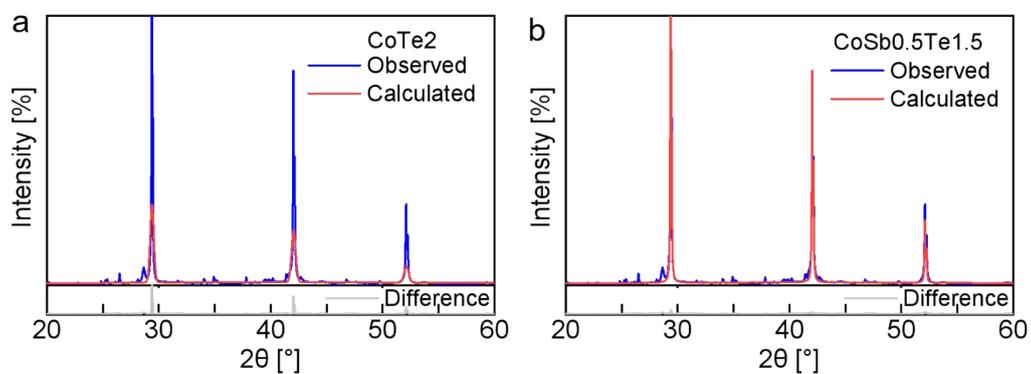


Figure S4 Rietveld refinement of the XRD pattern of AgSbTe_2 with CoTe_2 (a) and $\text{CoSb}_{0.5}\text{Te}_{1.5}$ secondary phase

Table S2 Parameter of CoTe_2 and $\text{CoSb}_{0.5}\text{Te}_{1.5}$ phase from Rietveld refinement

| Parameter | CoTe_2 | $\text{CoSb}_{0.5}\text{Te}_{1.5}$ |
|---------------------|-----------------|------------------------------------|
| a (Å) | 5.273 | 5.268 |
| b (Å) | 3.817 | 3.883 |
| c (Å) | 6.229 | 6.160 |
| V (Å ³) | 125.4 | 126.0 |