Supporting Information

Revealing self-aligned γ-SnTe ultrathin nanosheets in thermoelectric β-SnTe

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Figure S1. The single-phase polycrystalline \( \beta \)-SnTe sample. (a) A typical X-ray diffraction pattern of the Sn\(_{0.5}\)Te\(_{0.5}\) bulk sample. The scans were recorded in the range of \( 2\theta = 20-75^\circ \) with a step size of 0.02°. The X-ray diffraction pattern can be indexed as \( \beta \)-SnTe (\( Fm\bar{3}m \)) with a rock-salt structure. The calculated lattice parameter of \( \beta \)-SnTe is \( a=b=c=0.63621(3) \) nm. (b) and (c) Back-scattered electron scanning electron microscopy image and the corresponding energy dispersive X-ray spectroscopy (EDS) elemental maps of a polished Sn\(_{0.5}\)Te\(_{0.5}\) sample. The EDS results are consistent with the X-ray studies, indicating that the single-phase polycrystalline \( \beta \)-SnTe sample was obtained. Additionally, there is no apparent element enrichment at the grain boundaries in the Sn\(_{0.5}\)Te\(_{0.5}\) sample.
Figure S2. (a) HAADF-STEM image and (b,c) the fast Fourier transform (FFT) patterns of β-SnTe sample containing a nanosheet, viewed along the $[\bar{1}10]$ zone axis of β-SnTe. It is noted that the FFT-1 pattern is taken from the β-SnTe region containing the nanosheet, and the FFT-2 pattern from the perfect β-SnTe region. By comparing FFT-1 with FFT-2, the extra spots in the FFT-1 pattern can be discerned, as demonstrated by a yellow arrow in (b), resulting from the appearance of the γ-SnTe nanosheet in β-SnTe.
Figure S3. A schematic drawing of the \( \beta \)-SnTe region containing \( \gamma \)-SnTe nanosheet overlapped with the normal \( \beta \)-SnTe matrix, viewed along the (a) \([100]\) and (b) \([110]\) zone axis of \( \beta \)-SnTe. From the viewpoint of structural model, the overlapping of \( \beta \)-SnTe region containing \( \gamma \)-SnTe nanoscale precipitate (a\(_1\) and b\(_1\)) and the normal \( \beta \)-SnTe matrix (a\(_2\) and b\(_2\)) results in the superposed structure models (a\(_3\) and b\(_3\)), which matched well with the experimental HAADF-STEM images (a\(_4\) and b\(_4\)). In (b\(_1\)), two types of nanosheet/\( \beta \)-SnTe interface can be distinguished. If the \( \beta \)-SnTe part containing \( \gamma \)-SnTe nanosheet (b\(_1\)) is in the majority of the HAADF-STEM sample along the viewing direction, these two types of nanosheet/\( \beta \)-SnTe interface can also be discerned, as shown in the HAADF-STEM images (b\(_4\)). The interfaces are indicated by colored arrows in (b\(_1\)), (b\(_3\)), and (b\(_4\)).
Movie S1. The structure evolution of \( \gamma \)-SnTe ultrathin nanosheet to \( \beta \)-SnTe occurs under *in situ* electron-beam irradiation. The *in situ* electron-beam irradiation experiments were performed on a JEOL ARM200F microscope equipped with a probe aberration corrector, operated at 200 keV. Under the HAADF conditions, the video of the phase transition from \( \gamma \)-SnTe ultrathin nanosheet to \( \beta \)-SnTe was captured by recording the preview window during the experiments. In HAADF-STEM mode, the imaging conditions are a beam current of \( \sim 6.4 \) pA, a pixel dwell time of \( 37.8 \) \( \mu s \)/pixel and a pixel size of \( \sim 0.037 \) Å\(^2\), which corresponds to a radiation dose of \( \sim 4.1 \times 10^6 \) e/nm\(^2\). It is noted that the phase transition occurs in the course of the acquisition of time series consisting of 20 frames.