

Supplementary Information for “Surface oxidation and thermoelectric properties of indium-doped tin telluride nanowires”

1. Temperature profile

The actual growth temperatures versus position were measured using an external thermocouple. Zero inch corresponds to the center of the furnace where the precursor SnTe powder is located. The first substrate is placed between ~ 4 and ~7 inches, the second substrate is placed between ~7 and ~10 inches and the third substrate is placed between ~10 and ~13 inches. The high temperature zone is defined from 0 to 10 inches and the low temperature zone is between 10 inches and 13 inches.

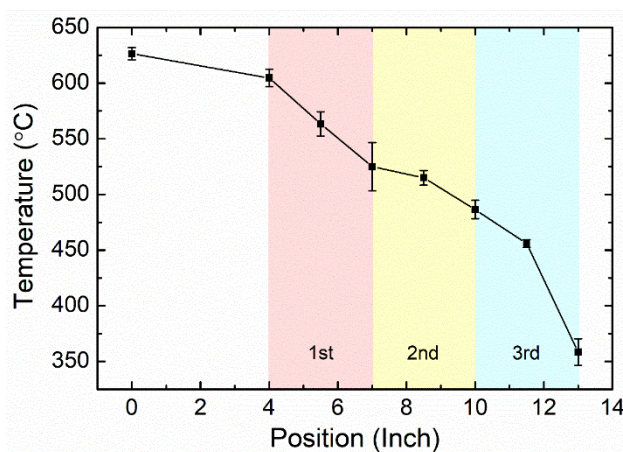


Figure S1. Temperature versus position of the actual growth. Shaded regions correspond to where different substrates were placed.

2. SEM images and EDX spectra of Au-Sn-Te alloy on the nanowires from all three substrates

Figure S2 shows the SEM images and EDX spectra taken from the tips of nanowires from the first, second and third substrate respectively. The peaks of Sn, Te and Au indicate that the particle on the tip of the nanowire is Au-Sn-Te alloy.

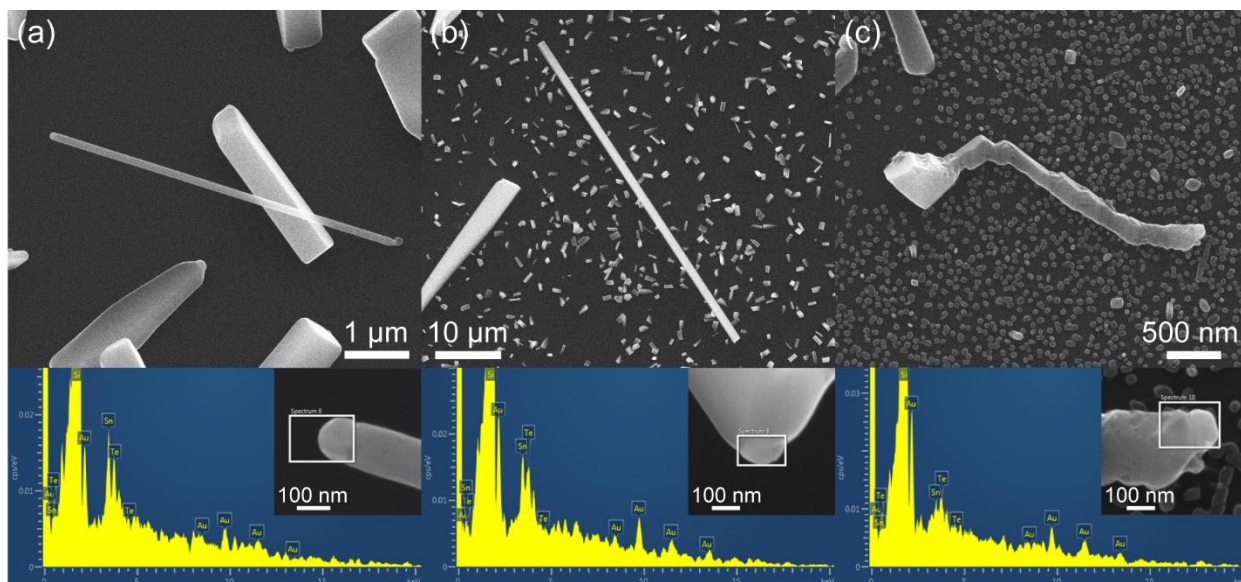


Figure S2. SEM images and EDX spectra taken from a typical nanowire from the (a) first, (b) second and (c) third substrate respectively. Insets are the magnified SEM images of the tips of nanowires where EDX was conducted.

3. SEM images and EDX spectra of nanowires from all three substrates

Figure S3 shows the SEM images and EDX spectra taken from the nanowires from the first, second and third substrate respectively. The peaks of Sn and Te are visible, but peaks of indium, detectable by XPS, are absent in the EDX spectra taken from nanowires on all substrates. A number of nanowires from each substrate are investigated by EDX, the average atomic ratio between Sn and Te in the nanowires is ~ 1.31 from the first substrate, ~ 1.13 from the second substrate and ~ 1.18 from the third substrate. The deviation of Sn/Te ratio from 1 is likely due to the large error bar in the EDX characterization, in particular when the spectrum is dominated by silicon signal.

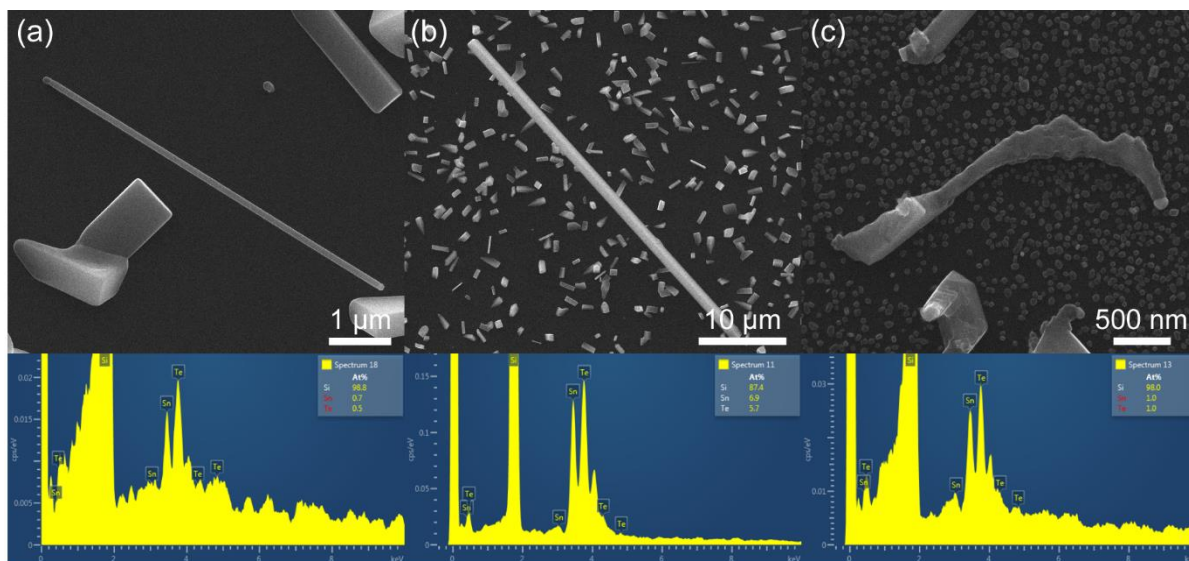


Figure S3. SEM images and EDX spectra taken from a typical nanowire from the (a) first, (b) second and (c) third substrate respectively. EDX was conducted on the body of the nanowires.

4. SEM images of a control growth at a lower temperature

The control growth was done at zone temperatures 480/600/425°C, other parameters were the same as the growth discussed in the main text. Figure S4a shows a straight and smooth nanowire at the first substrate. Figure S4b displays an SEM image taken from the right side of the second substrate, “twisted” nanowires are observed. “Twisted” nanowires are also present at the left side of the third substrate as shown in Figure S4c, the right side of the third substrate has no nanowires.

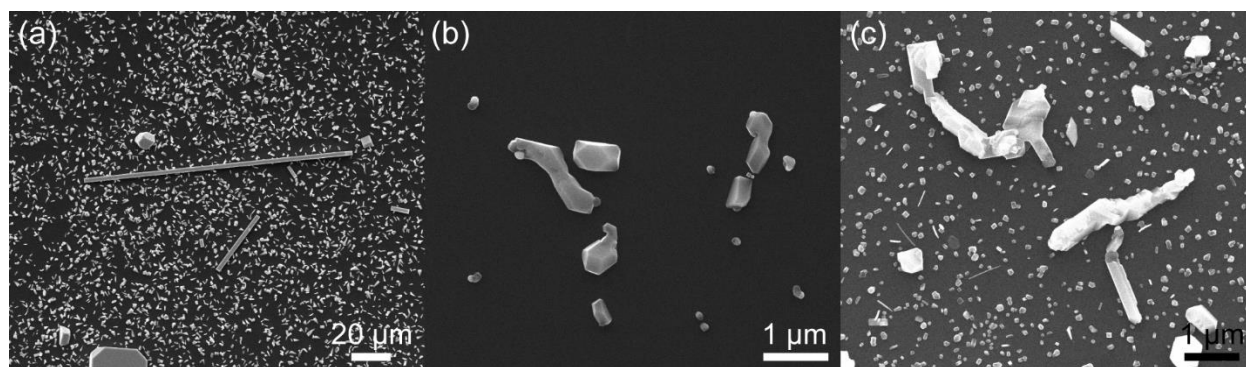


Figure S4. SEM images taken from the (a) first, (b) second, and (c) third substrate of the control growth respectively.

5. Similar results from X-ray photoelectron spectra taken at other spots on the first substrate before sputtering

Other three different spots on the first substrate were investigated by XPS before sputtering. The spectra after calibration against C 1s peak are shown in Figure S5. O 1s peak can be fitted by two components where one component with a higher binding energy corresponds to -2 oxidation state of SiO₂ while the other component is attributed to the surface oxides of SnTe. Sn 3d peaks corresponding to +4 oxidation state, Te 3d peaks corresponding to +4 and 0 oxidation states and In 3d peaks corresponding to +3 oxidation states are also observed. The results suggest that the sample surface is oxidized and forms In₂O₃, SnO₂, Te and TeO₂.

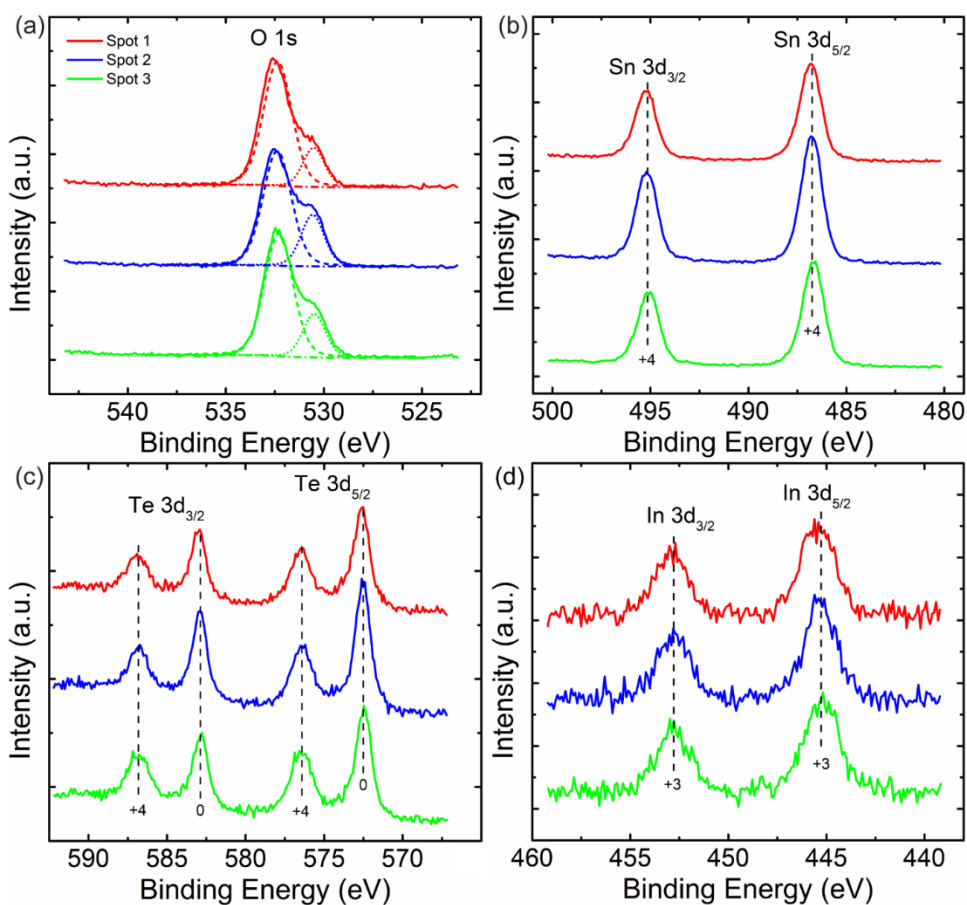


Figure S5. X-ray photoelectron spectra: (a) O 1s (b) Sn 3d (c) Te 3d and (d) In 3d core level spectra taken before sputtering from three different spots on the first substrate respectively. The spectra are vertically shifted for clarity. The dashed lines indicate roughly the peaks corresponding to different oxidation states. The oxygen peaks in Figure S5 (a) are fitted using two components.

Table S1 shows sample compositions determined based on X-ray photoelectron spectra taken at the three spots on the first substrate before sputtering. The atomic ratios of In: Sn: Te from different spots are similar to each other.

Table S1. Sample compositions at three different spots on the first substrate before sputtering

Spot number	In / Sn / Te
1	3.8/78.5/17.7
2	3.2/80.5/16.4
3	4/77.4/18.6

6. X-ray photoelectron spectra and quantitative analysis from three different spots on the second substrate

XPS measurements were carried out on three different spots on the second substrate, the corresponding spectra after calibration against C 1s peak are shown in Figure S6. The peak positions of O 1s, Sn 3d and Te 3d are similar as those obtained from the first substrate, indicating the presence of SnO₂, Te and TeO₂ on the sample surface. However, no In peaks were observed, suggesting the indium concentration is below the detection limit. Quantitative analysis of XPS data (Table S2) shows Sn-enriched surface as observed on the first substrate.

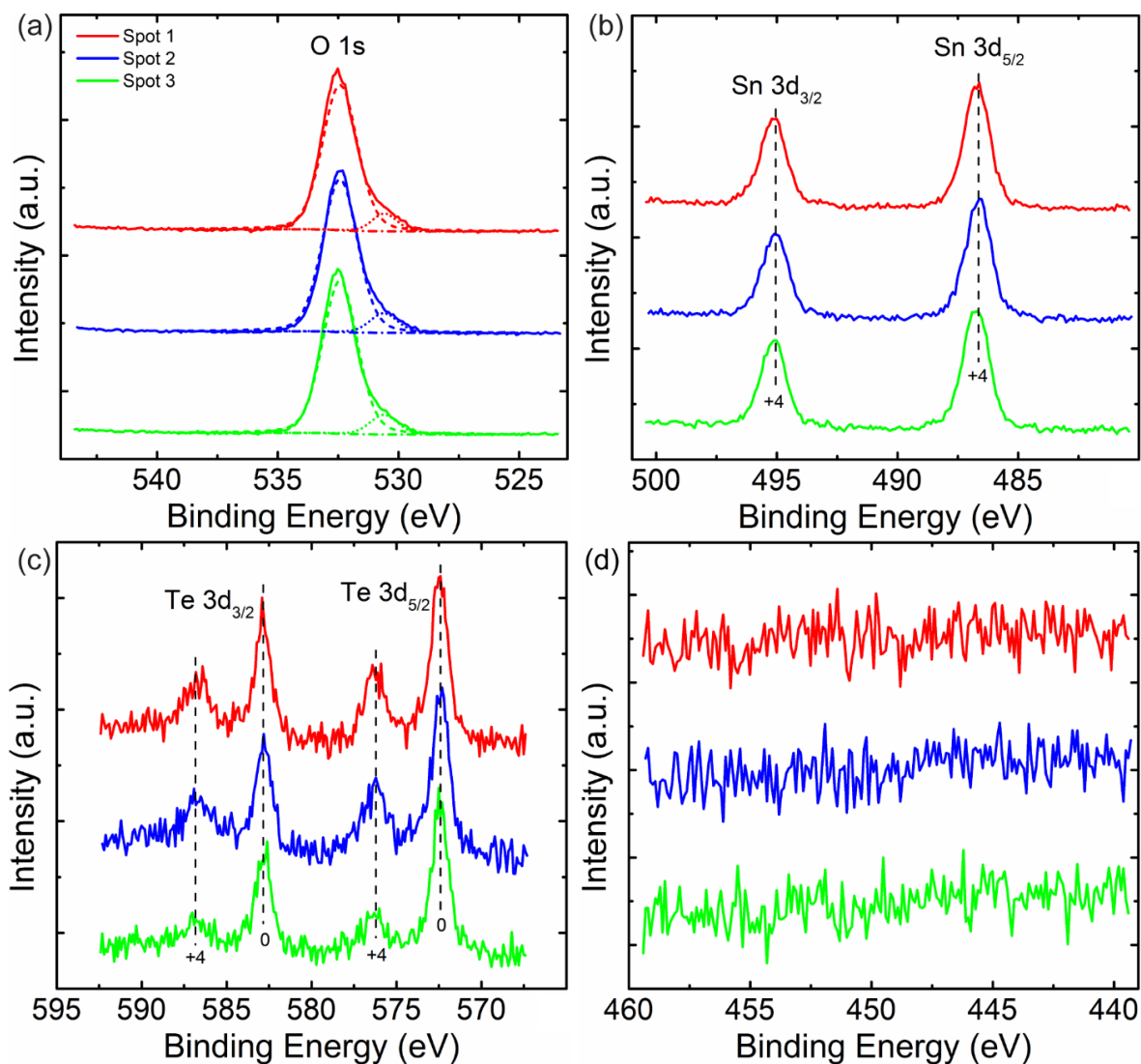


Figure S6. X-ray photoelectron spectra: (a) O 1s (b) Sn 3d (c) Te 3d and (d) In 3d core level spectra taken from three different spots on the second substrate respectively. The oxygen peaks in Figure S6 (a) are fitted using two components.

Table S2. Sample compositions at three different spots on the second substrate

Spot number	Sn / Te
1	82.3/17.7
2	80.1/19.9
3	85.1/14.9

7. X-ray photoelectron spectra and quantitative analysis from three different spots on the third substrate

X-ray photoelectron spectra were also taken at three different spots on the third substrate. Figure S7 shows the spectra after calibration against C 1s peak. Oxidation states of O, Sn, Te and In similar as that obtained from the first and second substrates are present on the third substrate. The component corresponding to surface oxides of SnTe in the oxygen peak appears comparable to the component from SiO₂. This can be caused by the large area coverage of the substrate surface by dense nanostructures. The intensity of +4 Te peak is stronger than 0 Te peak in this case.

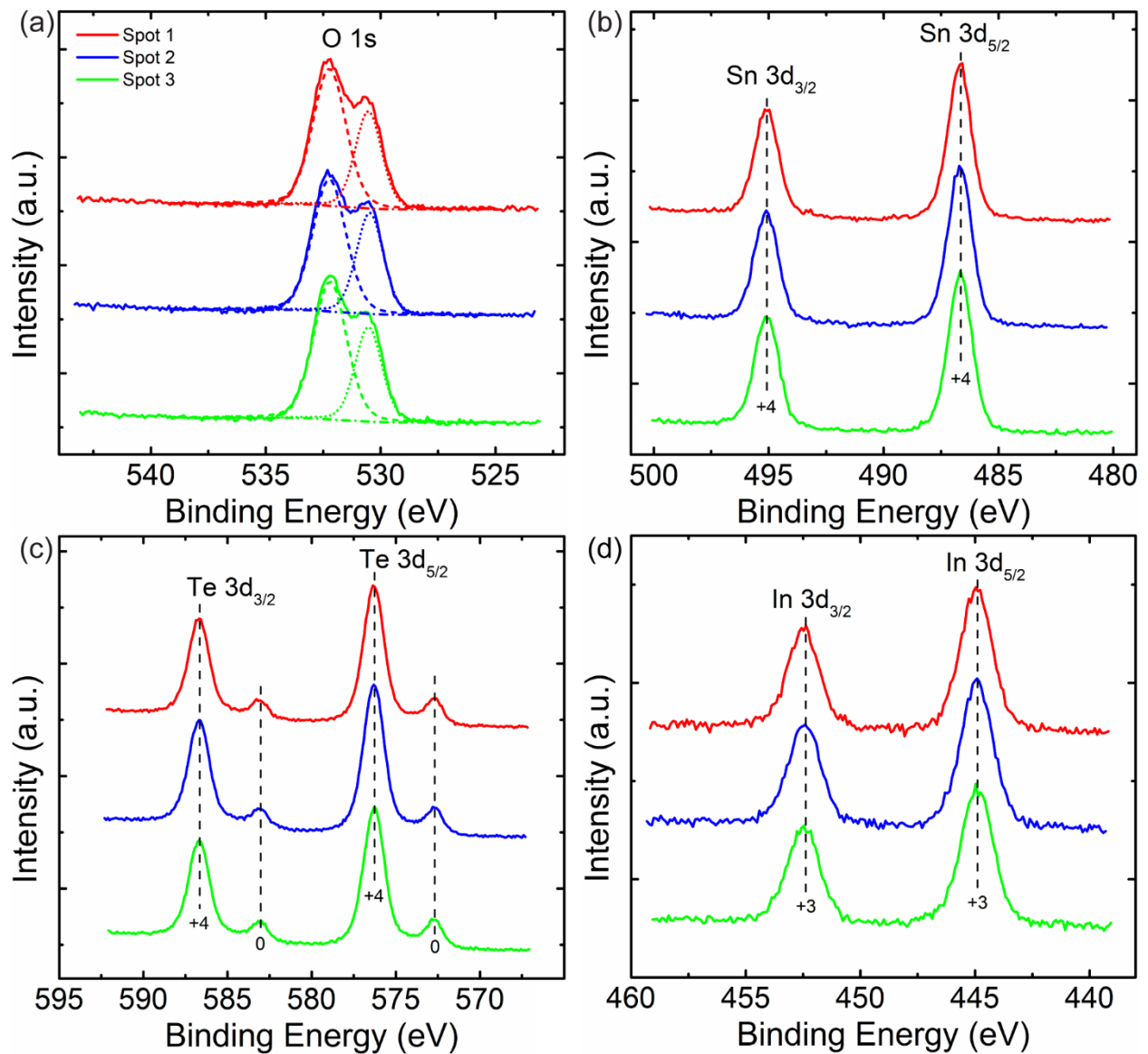


Figure S7. X-ray photoelectron spectra: (a) O 1s (b) Sn 3d (c) Te 3d and (d) In 3d core level spectra taken from three different spots on the third substrate respectively. The oxygen peaks in Figure S7 (a) are fitted using two components.

Table S3. Sample compositions at three different spots on the third substrate

Spot number	In / Sn / Te
1	9.1/41.6/49.3
2	8.7/40.6/50.7
3	8.5/42.2/49.3

8. SEM images of the nanowires and microcrystals from the first substrate after sputtering

After sputtering, the microcrystals appear etched on the facets exposed to argon, while the nanowires are thinned down along one side, resembling nanoribbons.

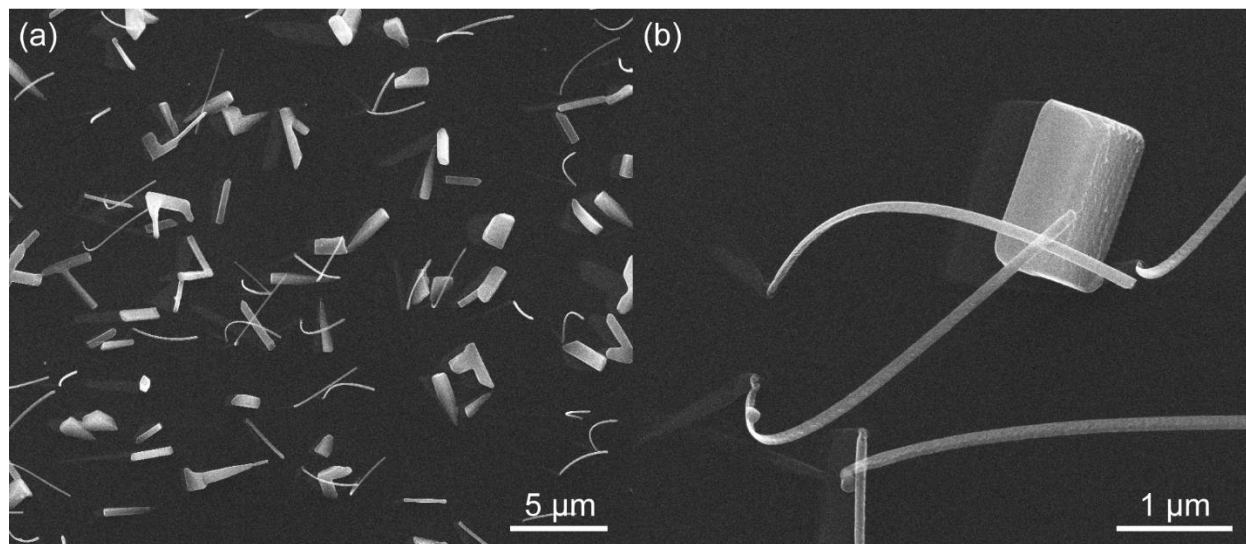


Figure S8. (a) SEM image of the sputtered area (b) Zoomed-in SEM image displaying sputtered microcrystal and nanowires.

9. An example of curve fitted Sn 3d_{5/2} and Te 3d_{5/2} spectra

For quantitative analysis, XPS data were fitted by the Gaussian-Lorentzian lineshape with a fixed Gaussian contribution of 80%. In Figure S9a, the black curve corresponding to Sn 3d_{5/2} is the fitted envelope treated using two components, Sn⁴⁺ (red) and Sn²⁺ (blue). In the case of Te 3d_{5/2} (Figure S9b), the data are fitted using three components, Te⁴⁺ (blue), Te⁰ (green) and Te²⁻ (red).

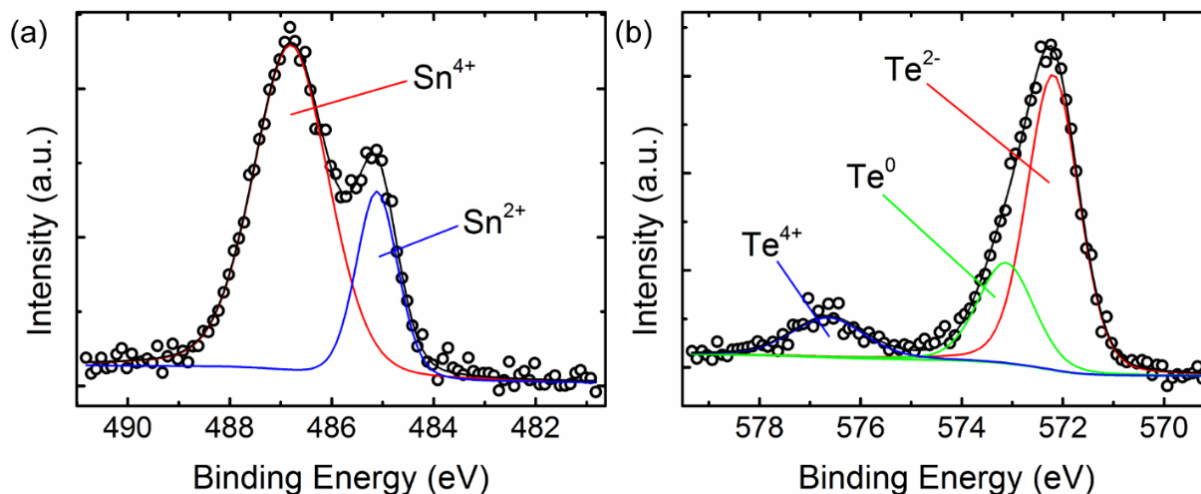


Figure S9. Representative fittings to the X-ray photoelectron spectra of (a) Sn 3d_{5/2} and (b) Te 3d_{5/2} respectively. The open circles are experimental data, black curves are curve fitted data and colored curves correspond to different components used for curve fitting.