THE OXIDATION PREVENTING CdTe- COATING OF $Pb_{1-x}Sn_xTe$ PENTAGONAL NANOWIRES GROWN BY MBE

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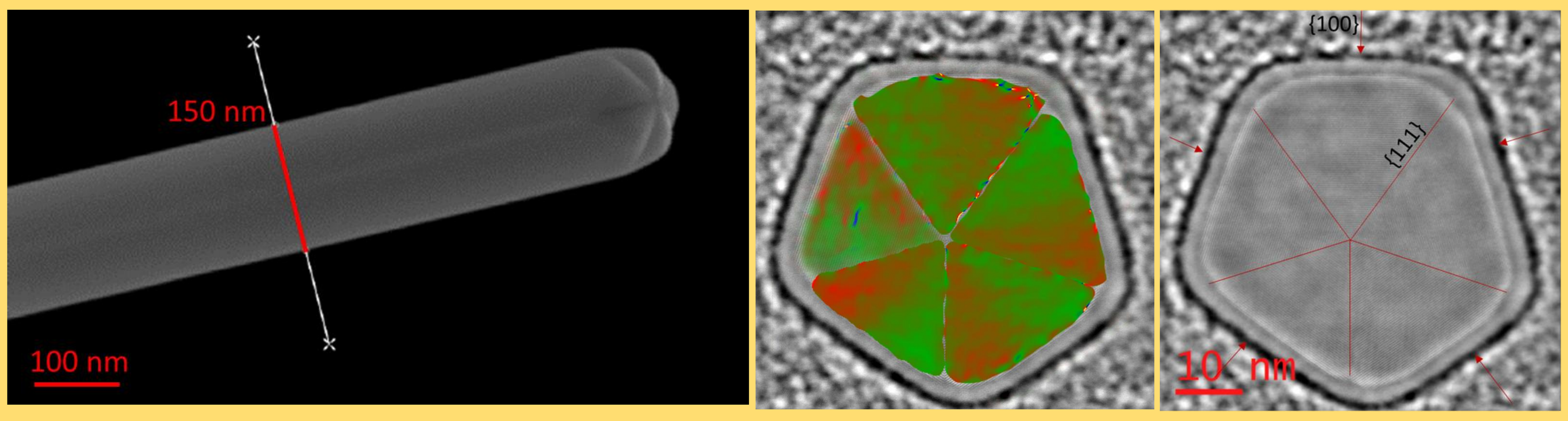
SnTe and $Pb_{1-x}Sn_xTe$ narrow gap semiconductors are interesting because of their thermoelectric and optoelectronic applications and topological crystalline insulator (TCI) properties [Xu et al., Nat. Comm. 2012], [Fu, Phys.Rev.Lett., 2011].

Here we present results of transmission electron microscopy (TEM) studies of molecular beam epitaxy (MBE) grown IV-VI nanowires (NWs). The FIB lift-off procedure was used to fabricate specimens for cross-section investigations. Ternary $Pb_{1-x}Sn_xTe$ NWs were grown on (100)- and (111)-oriented silicon substrates (w/wo catalyst). Apart from typical NWs with a square cross-section, unusual twinned NWs with 5 distinguishable segments were observed near x=0.5 [Hussain et al., Arxive 2024, arXiv.2401.03455]. Each segment exhibits a growth axis [110] and {111} plane boundaries between them.

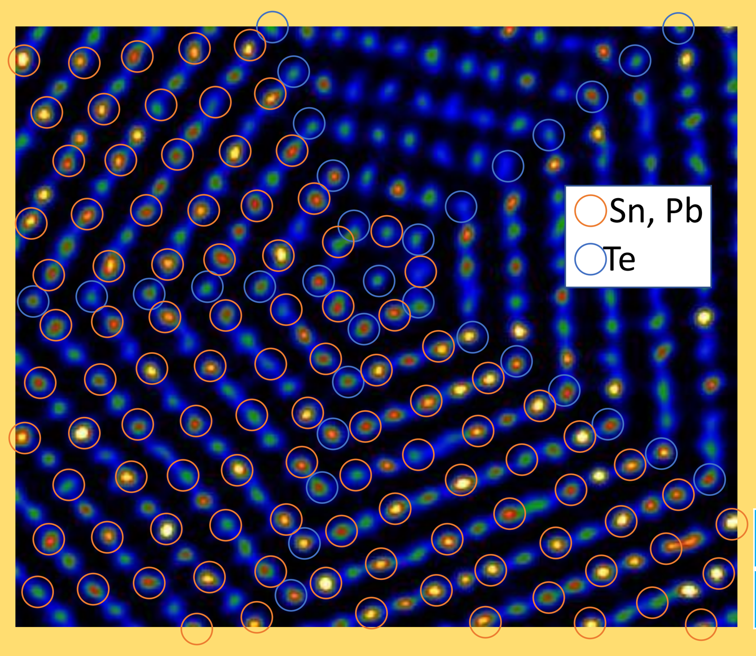
The chemical composition was examined by the energy-dispersive X-ray spectrometry (EDXS). Tin was found to migrate outward and surface oxygen (from surface oxidation) into the NW interior. Oxidation processes are detrimental to the prospective use of topologically protected surface states. Hence, methods to inhibit near-surface oxidation are crucial. In the case of rectangular NWs, the catalyst gold droplet was found to be a good oxidation inhibitor.

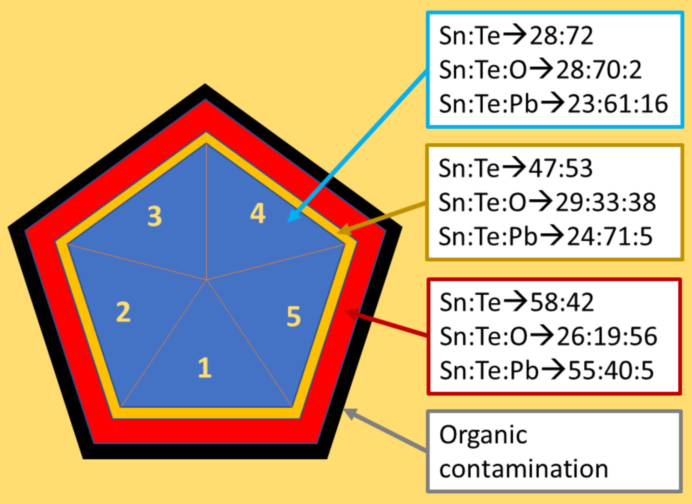
Another method investigated for pentagonal NWs was coverage of CdTe – insusceptible for oxygen. Attempts to grow the full CdTe shell led to epitaxial CdTe crystals forming thin pillars at five edges along the nanowire, into which twinning from the $Pb_{1-x}Sn_xTe$ core propagated. As expected, on the interface between rock salt $Pb_{1-x}Sn_xTe$, and the zinc blende CdTe, the misfit dislocation network was found.

Surface degradation in uncovered NWs



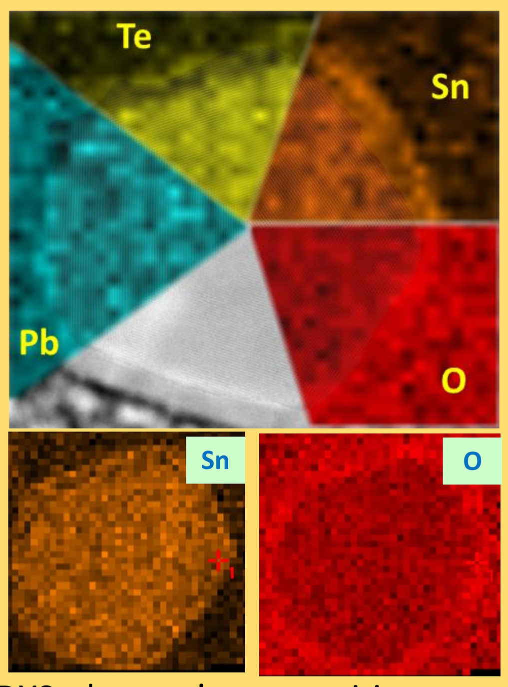
SEM images of 5-fold $Pb_xSn_{1-x}Te$. (left) Smooth and roundly shaped tip of the, (middle) GPAs' εyx rotation parameter, (right) perpendicular cross – section of the NW in the [110] zone axis.





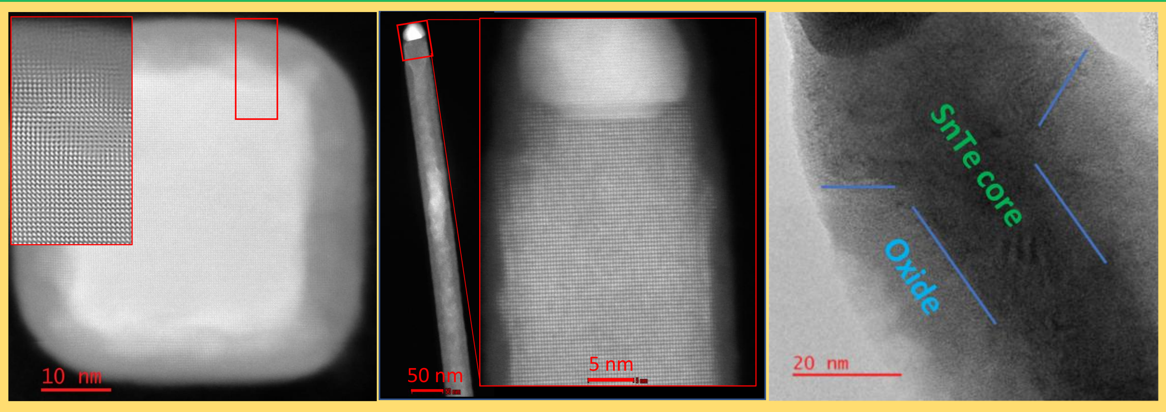
	1	2	3	4	5
Angle [deg.]	73.7	71.4	71.3	73.2	70.4

(left) Color coded intensity image of 5- fold $Pb_{1-x}Sn_xTe$ NW with identified Sn/Pb or Te atoms. (right) schematic picture of the cross- section of the NW with marked elemental ratios, and labeled measured angle in segments. Theoretical crystallographic angle between {111} planes is 70,53°.

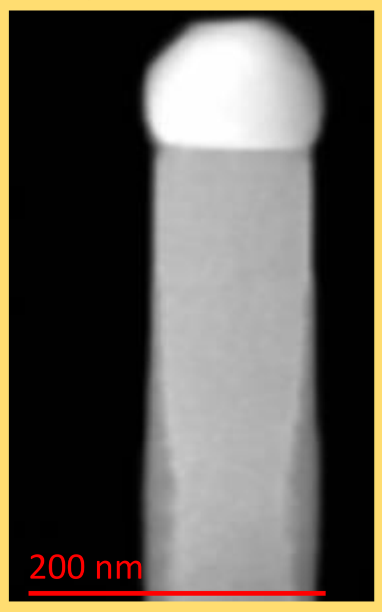


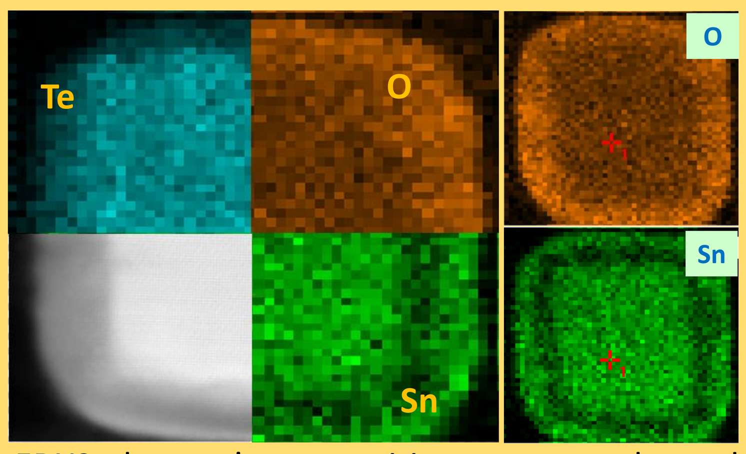
EDXS element's composition maps overlapped with STEM image (upper), with extracted maps for tin and oxygen respectively (lower two).

Surface degradation in 4 - fold NWs



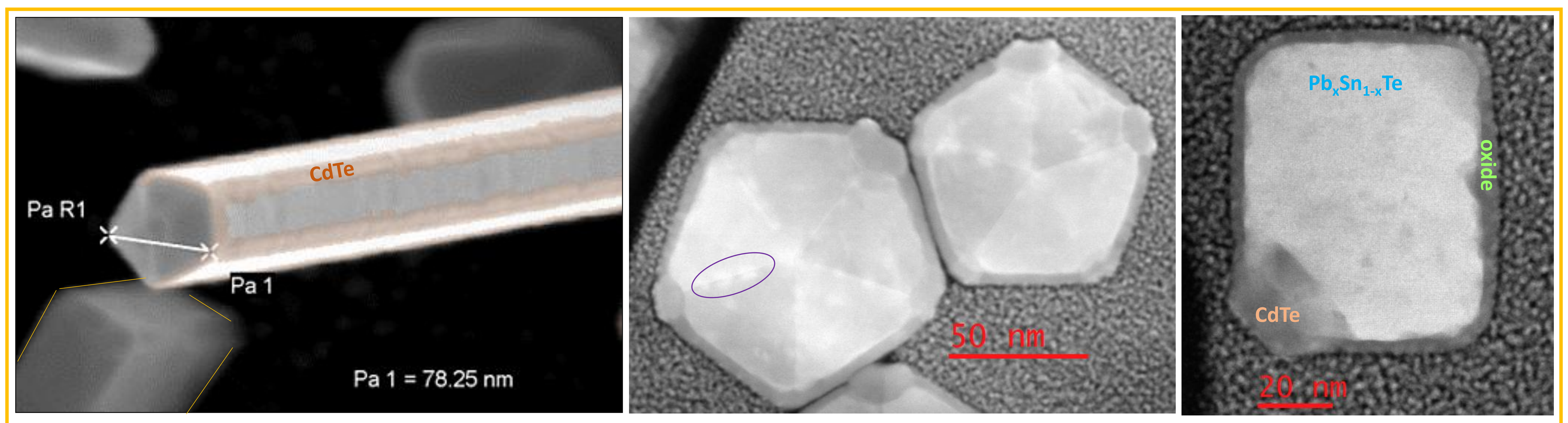
STEM image of cross – sectioned 4 – fold nanowire with visible rock – salt structure.
STEM image of tetragonal NW in planar wiev.
HRTEM image of protective capabilities of gold in the catalyzing droplet on top of the NW.



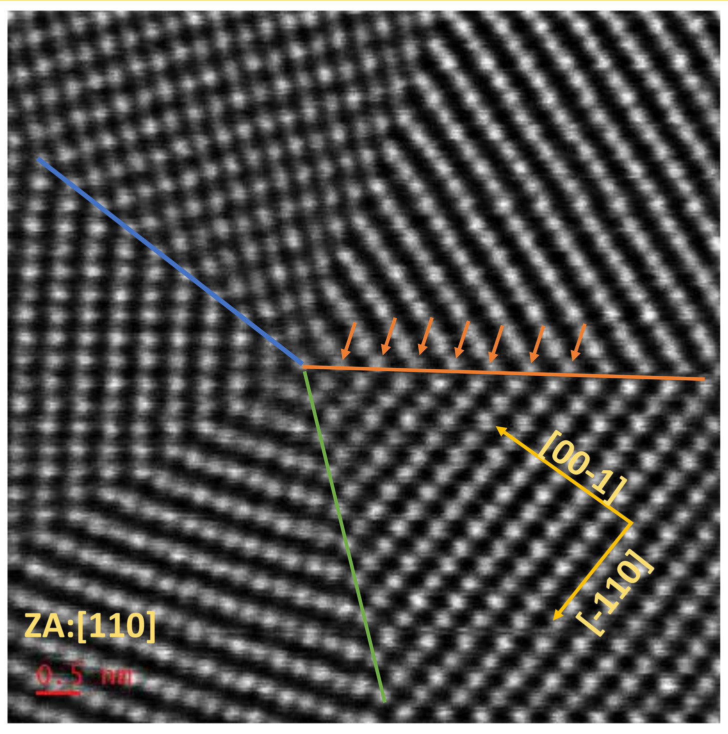


EDXS element's composition maps overlapped with STEM image (upper), with extracted maps for tin and oxygen respectively (lower two).

STEM image of SnTe NW with golden droplet on the top, and with Au incorporated in the NW's sidewalls. The protective properties gold can be seen.



SEM image of pentagonal PbxSn1-xTe with deposited CdTe. CdTe is marked in pinkish color.
STEM image of NWs cross-section, strain fields are marked with a circle.
STEM of a square cross-section of a typical IV-VI nanowire after CdTe deposition.

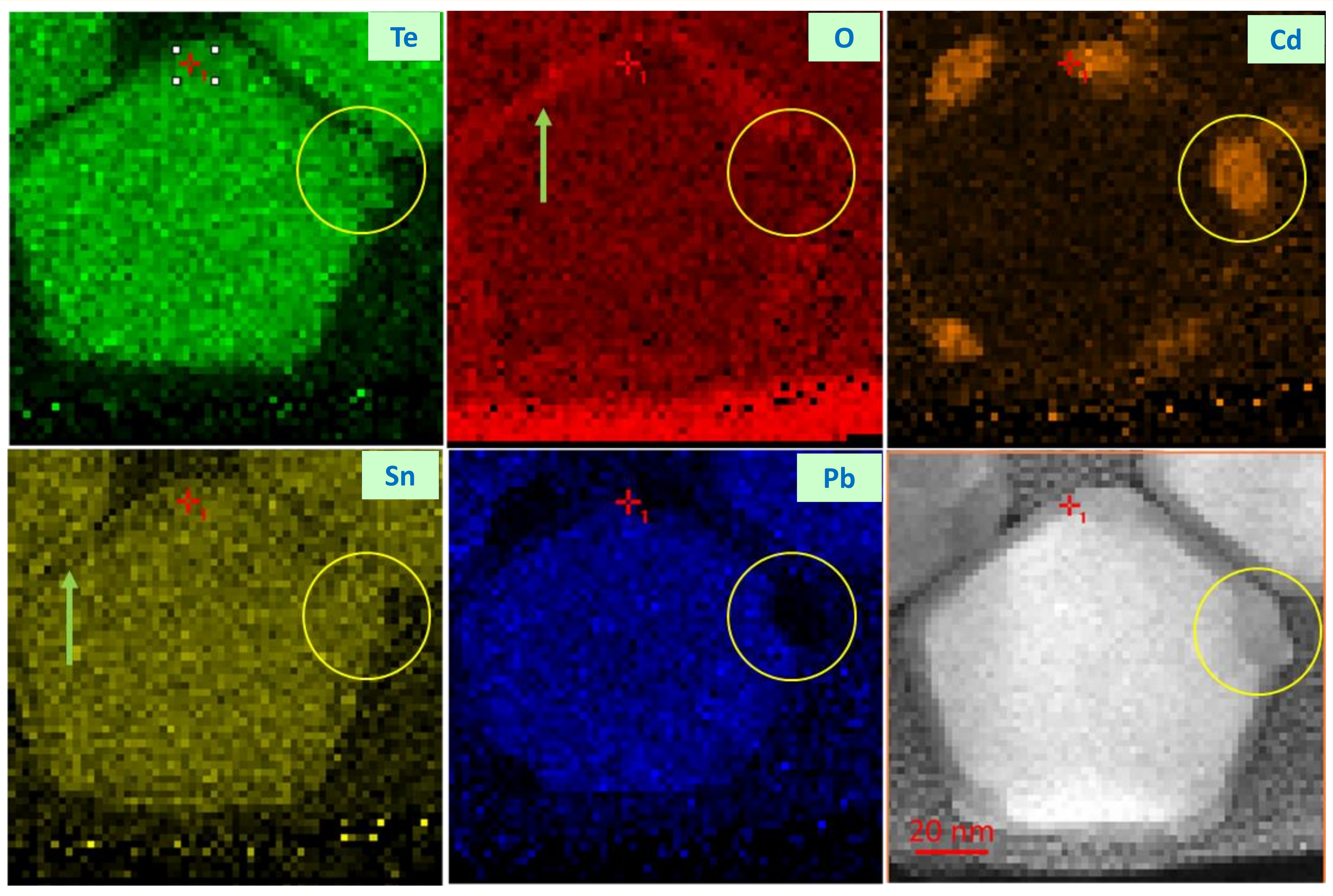


STEM Z-contrast image of 5- fold $Pb_{1-x}Sn_xTe$ nanowire with rock - salt crystal structure.

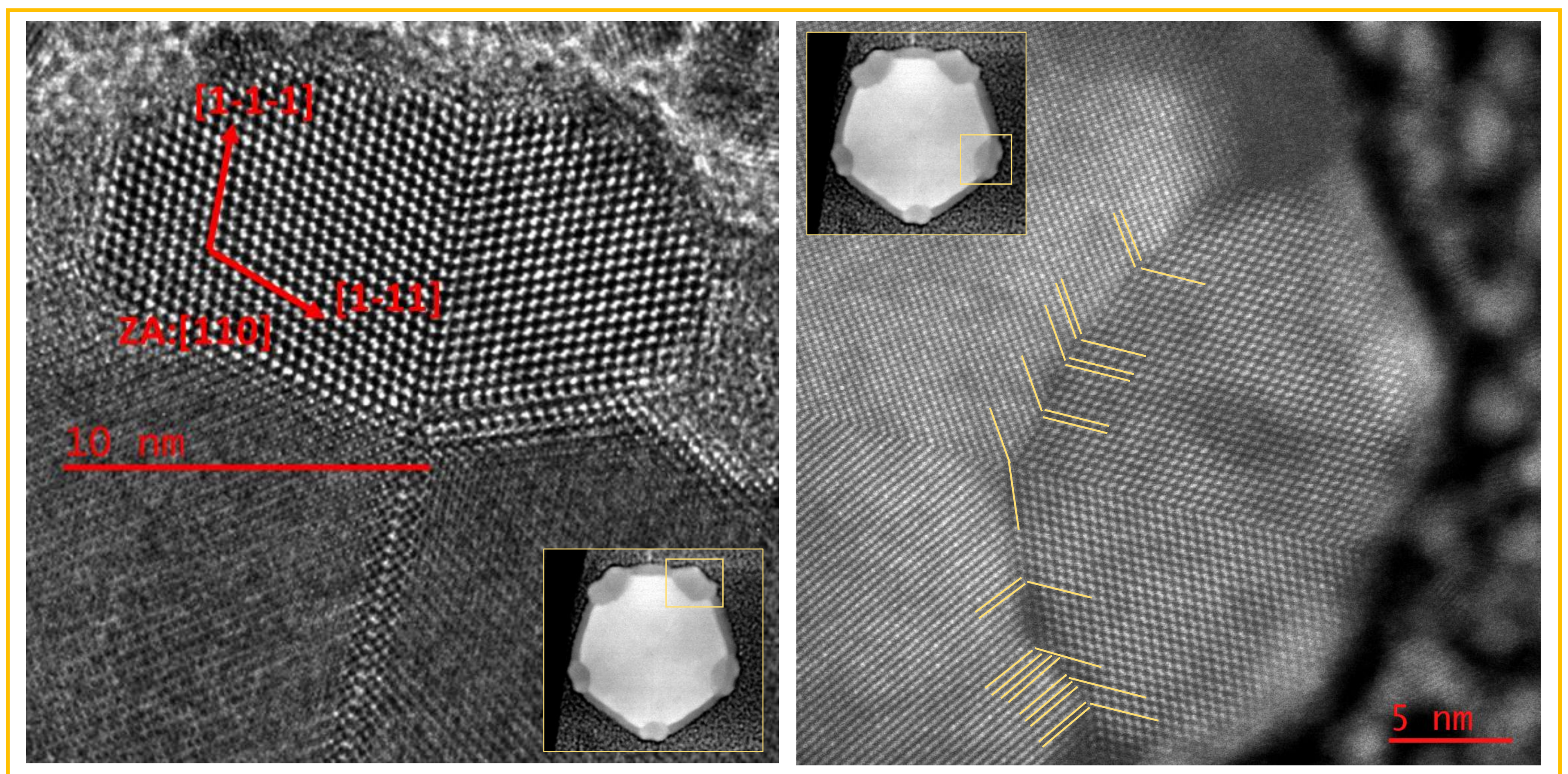
Blue line: normal contact twinning with mirror plane.

Orange line: twinning with contact displacement dislocation (one atom in a row on the boundary is misplaced).

Green line: misfitted twinning (rows of atoms are slightly misfitted in relations to each other).



EDS maps of elemental composition. Green arrows are pointing tin – depleted area associated with the genesis and composition of the oxide [Berchenko et al., Appl.Surf.Sci., 2018]. The yellow circle shows one of the NW's corners where the CdTe accumulates in the pillars.



HRESTEM filtered image of one of the CdTe „twin/bulb" (pillar's cross – section).
STEM image of the „twin/bulb". The misfit dislocations marked in yellow.

- We show the growth of NWs $Pb_{1-x}Sn_xTe$ in two possible forms – with square and (newly discovered) pentagonal cross – sections;
- Due to the presence of tin, the surface of the IV – VI materials is susceptible to oxidation;
- In NWs IV – VI, Sn and O migration processes are observed in the radial direction;
- Due to its crystallographic and electronic properties, CdTe is known to be a suitable protective coating for IV – VI NWs;
- In case of the IV – VI NWs, we observe a tendency for CdTe to form clusters in the corners of the NWs instead of the typical core – shell structures.

Poster made for EMAS 2024 - 14th REGIONAL WORKSHOP ON: The Edge of new EM and Microanalysis Technology

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