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The structure and oxidation mechanism of Pb_{1-x}Sn_xTe nanowires

grown by MBE method

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In these research we present results of Transmission Electron Microscope (TEM) studies of Molecular Beam Epitaxy (MBE)-grown IV-VI nanowires (NWs). $Pb_{1-x}Sn_xTe$ as well as SnTe NWs were grown on both (100)- and (111)-oriented silicon substrates. Contrary to square cross-section observed for binary IV-VI NWs, ternary $Pb_{1-x}Sn_xTe$ possess 5-fold twinned cross-section independently on the presence of catalyst. Using HRTEM and HRSTEM, the whole NWs transferred onto holey carbon film, were separately investigated. Specimens sectioned by perpendicular cross-section with Focused Ion Beam (FIB) were investigated using X- Ray Energy Dispersive Spectroscopy (XEDS) profiles and maps to obtain semiquantitative atomic distribution. The atomic structure of epitaxial [110]||[110] heterointerface between (zinc blend) CdTe and (rock-salt) $Pb_{1-x}Sn_xTe$ was investigated by HRSTEM and aberration corrected HRTEM.



Fig. 1. STEM images of 4-fold SnTe NWs catalyzed with Pb: planarly view on the left, and the cross-section with extracted rock- salt structure on the right.





Fig. 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 structure with marked elemental ratios, and labeled measured angle of each from 5 blocks. Crystallographic angle is 70,53° and the label shows- the blocks are strained.



Fig. 2. (a) mixed STEM image of 4-fold SnTe NW with the EDS elemental maps that clearly shows specific distribution of the elements in intentionally homogeneous structure; **(b)** simple schematic image of the cross- section of the structure with Sn to Te ratio in each layer.



Fig. 3. STEM image of 5-fold (Pb,Sn)Te nanowire **(left)** with extracted and filtered image of the zoom of the central point on the **right.** Telluride {111}

Fig. 5. (a) HRTEM **(b)** STEM image of the SnTe nanowire with gold catalyst droplet on the top, **(c)** enlarged region marked on (b) image with orange square. The protective properties of the Au droplet, and Au- sidewalls layer can be seen.

Summary:

The 4- fold SnTe NWs with the rock- salt structure were investigated. Specific distribution of O, Sn, and Te was found on the XEDS elemental maps, and that clearly shows **reactive diffusion mechanism** of the surface oxidation.

The cross-sectional TEM images shows that the growth direction was along [001] crystal axis in NWs with 4-fold symmetry, and [110] for each 5-fold $Pb_{1-x}Sn_xTe$ symmetry block.

These blocks forms {111} planes twin boundaries with Te atoms on the interfaces and in the center of the pentagon. The gold- doped crystal that appears in the sidewalls of the NWs (Fig. 5c) can prevent the significant amorphous oxide layer

grain plane marked with orange lines. The central atom of the whole structure





