MBE growth and structural properties of SnTe/CdTe and Pb_{1-x}Sn_xTe/CdTe topological layers

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IV-VI narrow-gap semiconductor solid solution $Pb_{1-x}Sn_xTe$ crystallizes in the rock-salt crystal structure with the lattice parameter varying from a=6.46 Å for PbTe to a=6.32 Å for SnTe and matching very well to zinc-blende II-VI semiconductor CdTe (a=6.48 Å). Good lattice matching but different crystal lattice, coordination number and chemical bonding result in a variety of high crystal quality nanostructures with atomically sharp interfaces observed, e.g. in PbTe-CdTe materials system known in thermoelectricity and infrared optoelectronics. Recently it was theoretically proposed and experimentally discovered that SnTe and Pb₁. _xSn_xTe (x>0.4) bulk crystals, known to possess inverted band ordering, are topological crystalline insulators (TCI). In contrast, CdTe is a semiconductor with topologically trivial band ordering. It offers an intriguing possibility of preparing high crystal quality epitaxial topological/trivial multilayers with varying (by design) relative contribution of topological interface states to the bulk of the crystals.

A series of SnTe and Pb_{1-x}Sn_xTe layers (x=0.36 - 0.76) were grown by molecular beam epitaxy (MBE) on GaAs (001) substrate with a thick CdTe buffer. Thickness of the layers, varying from 0.02 to 3 µm, was measured with scanning electron microscope (SEM, see cleaved cross-section, left panel below). By optimizing the temperature of growth and flux ratios of SnTe, Te, and Pb the optimal parameters were found to obtain single-phase high crystal quality films. During the growth films were monitored in situ by reflection highenergy electron diffraction (RHEED) to confirm the two-dimensional growth regime and crystal quality. The surface morphology was studied by atomic force microscopy (AFM, see right panel below) revealing atomic steps and roughness parameter of 1,7 nm for 4 µm² region. The lattice parameter, strain and degree of relaxation of SnTe layers were examined by X-ray diffraction method revealing, in particular, that SnTe layers are practically fully relaxed (relaxation degree about 96-98 %). An important physical parameter of SnTe and Pb_{1-x}Sn_xTe crystals is their non-stoichiometry that brings electrically active metal vacancies. We controlled this factor by Hall effect measurements revealing the expected very high hole concentration of about $p=10^{20}$ cm⁻³.

