Optical and Structural Properties of $Pb_{1-x}Sn_xTe$ Epitaxial Layers Grown on (001)-oriented CdTe/GaAs Hybrid Substrates

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$Pb_{1-x}Sn_xTe$ is a IV-VI narrow-gap semiconductor crystallizing in the rock-salt crystal structure with the lattice parameter varying in accordance with the Vegard law from a = 6.46 Å for PbTe to a = 6.32 Å for SnTe. Recently, it was theoretically predicted and experimentally demonstrated that both SnTe, and $Pb_{1-x}Sn_xTe$ (with $x > 0.4$) crystals possessing inverted band ordering are topological crystalline insulators [1–4]. The choice of CdTe (a = 6.48 Å) as a substrate was dictated by the fact that this compound is a wide gap topologically trivial material with a nearly perfect lattice match to PbTe and composition dependent small mismatch to $Pb_{1-x}Sn_xTe$.

In this work, we study optical reflectivity of $Pb_{1-x}Sn_xTe$ layers in the infrared range of spectrum with dominant optical dispersion due to plasma excitations of conducting holes. By experimentally determining the effective mass of carriers as a function of composition and temperature we expect to observe optical signatures of band inversion and topological transition.

A series of $Pb_{1-x}Sn_xTe$ layers were grown by molecular beam epitaxy on (001) – GaAs substrates with a several microns thick CdTe buffer layer. Thickness (0.02 μm – 3 μm) and composition ($x = 0.3 - 1$) of the $Pb_{1-x}Sn_xTe$ layers were determined by scanning electron microscope and X-ray spectroscopy, respectively. The lattice parameter, crystal strain, and $Pb_{1-x}Sn_xTe$/CdTe interface mixing were examined by high resolution X-ray diffraction and transmission electron microscopy techniques. Hall effect measurements revealed very high hole concentration of $p = 10^{19}\ cm^{-3} - 10^{20}\ cm^{-3}$, as expected for this alloy.

We carried out optical reflectivity measurements in the spectral range 0.1 eV – 0.5 eV and temperature range 10 K – 280 K, thus covering the plasma edge frequency for $Pb_{1-x}Sn_xTe$ layers with varying composition and hole concentration. In order to quantitatively analyze the spectra we applied a model of reflectivity from optical multilayer system. We accounted for plasma dispersion and layer thickness controlled interferences. The experimentally observed composition, temperature and carrier concentration dependent shift of plasma frequency is discussed in terms of band structure model of $Pb_{1-x}Sn_xTe$ with temperature and composition dependent inversion of conduction and valence bands.

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