Phase Transitions in Epitaxial Films of Ferroelectric Chalcogenides

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Abstract. Topological crystalline insulators are materials with inverted band structure where the surface states posses linear electronic dispersion, so called Dirac cones. There are even number of Dirac cones due to the inversion or mirror symmetry of the crystal structure. The inversion symmetry breaking can lead to an opening gap in odd number of the Dirac cones and transition of topological crystalline insulator to an ordinary \mathbb{Z}_2 topological insulator. That could be for instance achieved by a formation of surface charge region due to surface doping [1]. Another possible way to break down inversion symmetry is the combination of topological crystalline insulator with ferroelectric material.

The epitaxial thin films of chalcogenide alloy ferroelectric materials have been grown using molecular beam epitaxy on a BaF2 (111) substrates. We have studied two alloy systems of (Pb,Ge)Te and (Pb,Sn)Te. While PbTe has cubic structure at whole temperature range, GeTe is ferroelectric with Tc=700K and SnTe up to 110K, depending of the doping concentration. The pseudobinary alloys with varying concentrations allows us to tune the transition temperature. The ferroelectric materials have been studied using x-ray diffraction at low temperatures. The (Pb,Ge)Te films are showing clear structural phase transition in the lattice parameter, see Fig. 1(a). The intensity of odd diffraction peaks is very sensitive of the ferroelectric displacement of cationic and anionic sublattices. Thus, they allows us to evaluate absolute ferroeelectric displacement, see Fig2(b). The x-ray diffraction shows the Ge concentration dependence of the transition temperature, reaching 250K at 10% Ge concentration. On the other hand, low temperature x-ray diffraction of (Pb,Sn)Te did not reveal any structure change in the lattice parameter. While we have observed changes in Raman spectroscopy and also in EXAFS sopectroscopy, figure 1(d).



a)



FIGURE 1. (a) Out-of-plane lattice parameter of (Pb,Ge)Te. (b) temperature dependence of sublattice shift in (Pb,Ge)Te. (c) Out-of-plane lattice parameter of (Pb,Sn)Te. (d) Temperature dependence of the nearest neighbor distance of Sn atoms in (Pb,Sn)Te determined using EXAFS.

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